ANALYTICAL AND NUMERICAL STUDIES ON STRATIFIED FLUID FLOWS

by
Claudio Viotti

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Approved by:

Roberto Camassa
Richard M. McLaughlin
David Adalsteinsson
M. Gregory Forest
Brian L. White
Abstract

CLAUDIO VIOTTI: ANALYTICAL AND NUMERICAL STUDIES ON STRATIFIED FLUID FLOWS.
(Under the direction of Roberto Camassa and Richard M. McLaughlin.)

The mathematical modeling of stratified fluid flows is the overall subject of this work, which spans a range of more specific topics: internal gravity waves, shear instability, anomalous diffusion of passive scalars, vortex rings dynamics in stratified environments. This dissertation is organized in three parts.

Part I focuses on shear-induced instability in large amplitude internal waves. Previous studies have shown that an instability of the Kelvin–Helmholtz type can occur within internal wave-induced shear layers, leading to wave breaking and production of turbulence. It was also recognized that such wave breaking resembles the instability of parallel shear flows only superficially. This study aims to refine the understanding of shear-induced instability in this specific context, and to identify the mechanisms that eventually make the onset of shear instability for such flows a significantly more subtle mechanism than its parallel counterpart.

Part II is concerned with anomalous diffusive regimes for passive scalars advected in shear flows. The problem is studied from the standpoint of spectral analysis, which provides a natural way to classify diffusive regimes ensuing from different asymptotic limits in the governing parameters. The analysis identifies separate classes of eigen-modes, whose features dominate the evolution at different time and space scales in initial value problems with multiscale initial conditions.

Part III contains a numerical study of vortex ring dynamics in a stratified environment, which represents my contribution to a research project conducted at the UNC
Fluid Lab. Vortex rings made of fluid with density higher than the ambient fluid and propagating downward through a sharp density stratification are considered. Lab experiments have identified a critical phenomenon, which distinguishes the behavior of the falling vortex ring in either being fully trapped at the ambient density layer, or continuing through the layer in its downward motion. The numerical simulations presented are able to reproduce such behaviors and offer several details not visible in experiments.
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I thank my advisors, Roberto Camassa and Rich McLaughlin, from whom I have learned a great deal of science, and who made the years of graduate school a rewarding and pleasant experience.

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Part I

STABILITY OF PARALLEL AND WAVE-INDUCED NON-PARALLEL STRATIFIED SHEAR LAYERS
Chapter 1

INTRODUCTION

1.1 Internal gravity waves

Internal gravity waves, i.e., any form of wave propagation due to non-uniformity of the fluid density and presence of a gravitational field, are a common feature of geophysical flows. Indeed, the ocean and the atmosphere represent the most clear examples of stratified fluid media on the planet. Their stratification is mainly due to variations in salinity (ocean) and temperature (ocean and atmosphere), on which the density of water and air depends.

The existence of internal waves is a relevant fact in several scientific fields. In physical sciences, such as oceanography and meteorology, internal waves have been recognized to be primary agents for transport and mixing of physical quantities (e.g., energy, momentum, salinity, temperature) in the environment (see, e.g., [42]). Internal waves affect biological life as well, as they contribute to the transport of living organisms, nutrients, and pollutants. This fact makes them elements of interest also for marine biologists and ecologists.

The internal waves we consider in this work are close to those occurring in the ocean. Since the 1960’s the development in ocean instrumentations allowed to gather much quantitative information on internal waves [47]. It is now well-established that the length scales typical of oceanic internal waves are very large: the wave lengths span
from hundreds of meters up to kilometers, and the vertical amplitude is in the range of 20 – 200 meters (measured in terms of vertical displacements of isopycnals, i.e., density level sets). Satellite observations (see, for instance, [51]) demonstrate the presence of internal waves in numerous locations on earth since the early 1980’s.

From the oceanic data collected, it soon became clear that internal waves occurring in real-world conditions are typically highly non linear phenomena. As such, their mathematical study presents a considerable challenge, which has been undertaken by applied mathematicians over the last decades. The mathematical study of internal waves (as well as other kinds of hydrodynamic waves) has motivated the spawning of many reduced models for wave dynamics (KdV-type, Green–Naghdi-type, etc., see 1.3.2). In more recent times direct numerical simulations based on the full governing equations (Navier–Stokes, Euler, Boussinesq, see §1.3.1) have also assumed a major role in the study of internal wave dynamics. In the writer’s personal view, the best insight is obtained by using all approaches in a complementary way.

The research efforts spent on this subject have targeted several processes constituting the “life-cycle” of internal waves: generation, propagation, shoaling and breaking; see Helfrich & Melville [47] for a broad and fairly recent review of the subject. The work presented in this thesis is centered around the onset of shear-induced instability in large-amplitude internal waves, which is a cause of wave breaking. Due to the mixing and energy dissipation involved in the process, the roll-up instability is an element that must be properly incorporated in our understanding of internal wave dynamics. The conditions setting roll-up, or Kelvin–Helmholtz instability, in the context of internal waves are still unclear in many regards, despite shear instability represents a classic topic in fluid dynamics.

This part of the thesis has been organized as follows. The rest of this chapter sets the stage for the problem under investigation and provides theoretical background
on internal gravity waves. Due to the broadness of the subject, only the elements explicitly referenced in the rest of the work have been included. Chapter 2 contains an introduction to the second main ingredient of this research, i.e., the spectral theory for stratified parallel shear instability. The same chapter also contains original results filling certain gaps in the standard textbook theory, that rise on surface when the concepts of spectral stability are applied to the case of wave-induced shear layers. The elements presented in the previous two chapter are merged in chapter 3, which contains a study of the local spectral properties of a the non-parallel shear induced by large amplitude internal waves. This chapter has a mostly analytical character. Chapter 4 contains numerical experiments performed to study the response of internal solitary waves to small perturbation. Numerical data are presented, interpreted and discussed based on the analysis developed in the previous chapters. Chapter 5 contains further theoretical developments aiming to clarify numerical results presented in the previous chapter that demand refined analysis. This part is presented in a rather self-contained way, but its connection with the bigger picture is emphasized.

1.2 Shear instability in large-amplitude internal waves

One of the most striking visualizations of shear instability in oceanic internal waves is provided in the work by Moum et al. [77]. The echosounder image reported in that paper, collected off the Oregon coast, clearly shows vortical roll-ups developing along a solitary-like internal wave; this kind of evidence has attracted considerable attention on the study of internal wave stability. Recent laboratory experiments (Fructus et al. 2009, Carr et al. 2008, Troy & Koseff 2005 [40, 24, 98]) and direct numerical simulations (Carr, King & Dritschel 2011, Barad & Fringer 2010, Tiron 2009 [25, 9, 96]) have examined the billow roll-ups developing in the shear regions of the wave field, which have been attributed to the growth of Kelvin–Helmholtz instability for wave-
induced stratified shear flows. One focus of these investigations has been to provide semi-empirical criteria, based on linear stability of these shear flows and direct observations, to be used as an organizing tool for the observations of instability.

Global-mode (discrete spectrum) stability analysis of internal waves has been previously attempted by means of direct computation, as in Pullin & Grimshaw [80], under the two-layer fluid assumption. They found numerically three-dimensional (slow) modulational instability for moderate-amplitude waves, and, for large-amplitude waves, (fast) Kelvin–Helmholtz instability. However, among their conclusions they emphasized that their results, even though insightful, are hardly valid for the finite-thickness interface case, especially in the regime dominated by the Kelvin–Helmholtz instability. We note that more recent work (Kataoka 2006) provides considerable evidence that only convective instability is present for internal waves in regimes of interest in typical oceanic applications.

For slowly varying shear flows, such as those occurring in jets, wakes, and boundary layers, a substantial amount of literature has been devoted to the issue of their stability, see, e.g., Crighton & Gaster (1976), Belan & Tordella (2006), Diamessis & Redekopp (2006) [31, 11, 33]. In this respect, analytic approaches have been developed making use of the slowly-varying flow assumption (which leads to a WKBJ analysis). This would seem a natural route to pursue in our case of internal wave-induced shear as well, and in fact the application of such theories has proven useful for seeking frequency and growth rate of unstable global modes in open shear flows (Monkewitz, Huerre & Chomaz 1993). However, as we shall see in this work, there are difficulties in the application of this approach to the case of internal waves with thin pycnoclines.

The above brief review completes our preliminary outline of the subject. We shall proceed, in the next section, with a summary of the mathematical background necessary to model internal waves.
1.3 Mathematical modeling of non linear internal waves

This section sets out in a concise way the basic background of governing equations and set-up employed to model internal gravity waves.

1.3.1 Governing equations

In this study we consider two-dimensional (2D) inviscid stratified incompressible fluids. The full governing equations is then represented by the variable-density Euler system

\[
\begin{align*}
(\rho u)_t + (u \cdot \nabla) (\rho u) &= -\nabla p - g \rho y, \\
\rho_t + u \cdot \nabla \rho &= 0, \\
\nabla \cdot u &= 0.
\end{align*}
\] (1.1)

The first equation represents conservation of momentum, the second is the density transport equation, and third expresses the incompressibility condition. The quantities \(u\) and \(\rho\) denote the fluid velocity and density respectively, \(p\) is pressure, and \(g\) is the gravity acceleration constant along the \(y\)-direction indicated by the unit vector \(y\). Subscripts denote partial derivatives with respect to time \(t\), \(\nabla\) is taken with respect to the standard Cartesian coordinates \(x = (x, y)\). When the density \(\rho\) presents only small variations about a reference value, i.e., \(\rho(x, t) = \rho_0 + \tilde{\rho}(x, t)\) with \(|\tilde{\rho}| \ll \rho_0\), it is legitimate to replace the above Euler equation with the simpler Boussinesq equations

\[
\begin{align*}
\dot{u}_t + (u \cdot \nabla) u &= -\frac{1}{\rho_0} \nabla \tilde{\rho} - g \tilde{\rho} y, \\
\tilde{\rho}_t + u \cdot \nabla \tilde{\rho} &= 0, \\
\nabla \cdot u &= 0.
\end{align*}
\] (1.2)
which are obtained by neglecting density variations in the inertial terms, and subtracting off the constant hydrostatic pressure \( \tilde{p} = p - g\rho_0 y \) (see for instance [56]). The Boussinesq approximation will be used in the spectral analysis of stratified shear flows (see Chapter 3), and in the energy balance for perturbed wave flows (in §4.2.1). The full Euler system will constitute the governing equations elsewhere.

In this work we shall always consider fluid domains consisting of horizontally unbounded regions, confined between two horizontal rigid walls, where the slip-wall no-penetration condition applies. This is a suitable numerical model for making comparisons with laboratory experiments performed in wave tanks, a good number of which is available in literature (see §1.2). Effects related to viscosity and molecular diffusivity of the scalar concentration responsible for density variations are neglected, consistently with approximations based on the typical temporal and spatial scales of internal wave propagation in experimental and geophysical situations of interest. All quantities in this work will be dimensional and expressed in SI units (m, s, kg), and the parameters we use in all our examples will match the typical magnitudes encountered in lab experiments.

1.3.2 Reduced models

Several reduced models have been developed to describe hydrodynamic waves, a comprehensive account can be found, for instance, in Whitam’s book [102]. Wave models can be grouped into two categories: weakly and strongly nonlinear. To the first category belong the well-known Korteweg–De Vries and Boussinesq equations. Such models represent asymptotic equations in the joint limit of small amplitude and long wave, whereby linear dispersive effects balance quadratic nonlinearity. To the second category belong the Green–Naghdi type models, which include the Choi–Camassa system for shallow-water internal waves. Such models are derived from a long-wave
limiting procedure, while no assumption is made on the wave amplitude. The Choi–Camassa version of the Green–Naghdi system is the most relevant model for this work, and will be briefly presented in the rest of this section. (For a full derivation the reader is referred to [29].)

The set up consists into an horizontally unbounded wave tank confined between top and bottom rigid lids. We assume a scaling in which the total height of the channel is unitary. The undisturbed stratification, i.e., the conditions prior to any wave generation, consists in two constant density layers of thickness $h_1$ and $h_2$ respectively. The location of the interface is represented by the function $\zeta = \zeta(x, t)$, its displacement relative to the unperturbed configuration is $\eta = \zeta - h_1$. The time dependent thicknesses of each layer is denoted by $N_1$ and $N_2$. The set of equations governing such two-layer system under the long wave approximation is

$$\begin{align*}
N_{1t} + (N_1 \overline{u}_1)_x &= 0, \\
N_{2t} + (N_2 \overline{u}_2)_x &= 0, \\
\overline{u}_{1t} + \overline{u}_1 \overline{u}_1 + g \eta_x &= -\frac{1}{\rho_1} P_x + \frac{1}{N_1} \left( \frac{1}{3} N_1 G_1 \right)_x, \\
\overline{u}_{2t} + \overline{u}_2 \overline{u}_2 + g \eta_x &= -\frac{1}{\rho_2} P_x + \frac{1}{N_2} \left( \frac{1}{3} N_2 G_2 \right)_x,
\end{align*}$$

Figure 1.1: Schematics of the two-fluid system with main notation definitions.
where \( \overline{u}_1 \) and \( \overline{u}_2 \) denote the layer-averaged horizontal velocities

\[
\overline{u}_1(x, t) \equiv \frac{1}{N_1} \int_{\zeta}^{1} u(x, y, t) dy, \quad \overline{u}_2(x, t) \equiv \frac{1}{N_2} \int_{0}^{\zeta} u(x, y, t) dy,
\]

\( P \) is the pressure at the interface, and the nonlinear dispersive terms are defined by

\[
G_1(x, t) \equiv \overline{u}_{1xt} + \overline{u}_1 \overline{u}_{1xx} - \overline{u}_{1x}^2, \quad (1.7)
\]

\[
G_2(x, t) \equiv \overline{u}_{2xt} + \overline{u}_2 \overline{u}_{2xx} - \overline{u}_{2x}^2. \quad (1.8)
\]

For solutions possessing a typical longitudinal wave length \( L \gg 1 \) (set for instance by the initial data) the above system is asymptotically accurate up to \( O(\epsilon^4) \) errors, being \( \epsilon = 1/L \).

### 1.4 Solitary waves

There seems to be general consensus on the fact that large-amplitude oceanic internal waves are close to solitary waves. Solitary waves are an important class of wave phenomena arising from the interplay between nonlinearity and dispersion. They are found in different areas of physics; the most notable examples are perhaps found in nonlinear optics and hydrodynamics.

Hydrodynamic solitary waves consist of non-linear traveling solutions of the Euler equations (1.1), propagating at constant speed \( c_W \). In particular, the waves we consider are large perturbations of a quiescent stably-stratified state which is recovered in the far field, \( \rho(x, y, t) = \bar{\rho}(y) \) in the limit \( |x| \to \infty \). The last condition defines solitary waves as localized disturbances, in contrast to other kinds of traveling waves such as Cnoidal waves (non-linear periodic wave trains). By using the traveling-wave ansatz inside (1.1) it is possible to derive a nonlinear elliptic equation, the Dubreil-Jacotin–Long (DJL) equation (see, e.g. Yih’s monograph [103], p. 104), which is the starting
point for numerical computations.

1.4.1 DJL equation

The stratified Euler equations possess non linear solutions consisting of waves traveling at constant speed \( c_W \) with frozen shape. We consider the case of a domain unbounded in the horizontal direction \( x \), confined between flat rigid lids at the top and bottom. By choosing to work in the wave frame we consider the wave as a steady flow with a uniform asymptotic current, i.e. \( U = -c_W \) and \( \psi = -c_W y \) as \( |x| \to \infty \). By using the fact that, in steady flows, \( \rho = \rho(\psi) \), it is possible to obtain a closed problem in a single independent variable. This is known as the Dubreil-Jacotin-Long (DJL) equation (for a derivation see, for instance, Benjamin [14]), that in terms of streamfunction \( \psi(x, y) \) reads

\[
\rho(\psi) \nabla^2 \psi + \rho(\psi) \left( gy + \frac{1}{2} |\nabla \psi|^2 \right) = \rho(\psi) \left( \frac{g\psi}{c_W} + \frac{1}{2} c_W^2 \right). \tag{1.9}
\]

The above equation identifies a one-parameter family of solutions in \( c_W \). The function \( \rho(\psi) \) must be prescribed and corresponds to the asymptotic stratification.

A numerical method to compute streamwise-periodic solutions from the DJL equation is described by Turkington et al. [99]. (Such method is referred to as TEW henceforth.) For the purpose of numerical computations the domain size must clearly be finite, and appropriate boundary conditions must be employed in the \( x \) direction. The periodic conditions employed by Turkington et al. are a suitable choice, as for large enough domains the computed waves approach the limit of solitary waves, which is the condition of interest in this work. A example of a solution of equation (1.9) is reported in figure 1.2.

Under the Boussinesq approximation the DJL equation reduces to the simpler form
(see, e.g., [15])

\[
\nabla^2 \psi + g \rho \psi (y - \frac{\psi}{c_W}) = 0.
\]

(1.10)

Even though in this study we always consider small relative density variations, we shall always use the full form (1.9) of the DJL equation.

All numerical simulations that will be presented next (§4.2) are based on the full Euler equations (1.1), and in particular all solitary wave solutions for the background states are computed without the so-called Boussinesq approximation of neglecting density variation in the fluid inertia. However, this approximation is compatible with perturbative expansions around the travelling wave background state, and it will be used for the analysis of these perturbations.

1.4.2 Green-Naghdi solitary waves

The long-wave model [29], often referred to as the Green-Naghdi approximation (actually developed earlier by [91]), allows to determine the interface displacement \( \eta \) as the solution of the nonlinear differential equation (in comparing with [29], equation (3.51), notice that in our non-dimensional units \( g = 1 \))

\[
(\eta_x)^2 = \frac{3(\rho_2 - \rho_1)}{c_{GN}(\rho_1 h_1^2 - \rho_2 h_2^2)} \frac{\eta^2(\eta - a_-)(\eta - a_+)}{\eta - a^*},
\]

(1.11)

where \( \eta \) is the interface displacement, and

\[
a_+ = \frac{h_1 h_2 (\rho_1 h_1 + \rho_2 h_2)}{\rho_1 h_1^2 - \rho_2 h_2^2}, \quad a_- = -q_1 \pm \frac{q_1^2 - 4q_2}{2},
\]

\[
q_1 = -c_{GN}^2 - h_1 + h_2, \quad q_2 = -h_1 h_2 \left( \frac{c_{GN}}{c_0} - 1 \right),
\]

\[
c_0^2 = \frac{h_1 h_2 (\rho_2 - \rho_1)}{\rho_2 h_1 + \rho_1 h_2},
\]

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with $h_2 \equiv \zeta_\infty$, $h_1 \equiv 1 - h_2$, and $\eta \to 0$ as $|x| \to 0$ for solitary waves. The relation

$$c_{GN}^2 = c_0^2 \frac{(h_1 - a)(h_2 + a)}{h_1 h_2 - a c_0^2}$$

is used to seek solitary waves with a given maximum interface displacement (for a wave of depression) $a \equiv \min(\eta)$. In order to solve (1.11) either standard numerical routines, or closed-form implicit solutions $x = E(\eta)$ involving elliptic integrals can be employed. We refer the reader to [29] for details. An example of solitary wave obtained by solving (1.11) is reported in figure 1.2, which also offers a comparison with a solution of the DJL equation (1.9) for continuous stratification.

A remark is in order at this point: solitary waves obtained by solving (1.11) are genuine long wave asymptotic approximations of their counterparts from the parent Euler two-fluid system only under certain conditions. As $a_- \to a_+$ the amplitude of solitary wave solutions tends to the limit $\min(\eta) = -q_1/2 \equiv a_m$, with $a_+, a_- \to a_m$. In the scaled coordinate $X = \epsilon x$ the right-hand side would be a $O(\epsilon^{-2})$ quantity, unless $\eta - a_m$ is a small $O(\epsilon)$ quantity itself. This implies that the long-wave asymptotics on which the model is constructed are regular asymptotics around the crest for near-maximum amplitude waves, but singular away from it, i.e., in the ‘flank’ regions of the wave. This agrees naturally with the fact that solitary waves become broader and flatter around the crest as the amplitude approaches its limiting value, while the flanks conserve an independent length scale. The wave flanks are effectively “internal layers” of the $\epsilon$-expansion performed in [29], using the terminology of singular perturbation theory [54]. (This terminology is only used here in the context of asymptotic analysis, and should not be confused with the analog for fluid stratification, i.e., the pycnocline.)

The Green-Naghdi model provides approximation for the velocity field in the outer
Figure 1.2: Comparison between a solitary wave in a continuous sharp stratification and a Green–Naghdi solitary waves that matches the maximum displacement of the mean-density isoline. Such isolines are referenced by the blue (continuous stratification) and red-dashed (Green–Naghdi) lines. The solitary wave in continuous stratification is computed using the TEW algorithm, the grayscale map represents the corresponding density field. The background stratification is set as described later in §4.1.1, with $\rho_1 = 1$, $\rho_2 = 1.02$ and $\delta = 1/16$. The wave speed is $c_W = 0.212$, which corresponds to a wave approaching the propagating front limit.

layers, which at leading-order is (in scaled variables)

$$ U_1(X) = c_{\text{GN}} \frac{h_1}{1 - \eta(X/\epsilon)}, \quad U_2(X) = c_{\text{GN}} \frac{h_2}{\eta(X/\epsilon)}. $$

Finally, $\eta(X)$, $U_1(X)$ and $U_2(X)$ can be employed as the outer layer solution and provide a solution accurate up to $O(\delta, \epsilon)$ errors under the restrictions remarked above, so that

$$ \zeta^{(0,0)}(X) \equiv \eta(X/\epsilon) + \zeta_\infty. $$
A detailed knowledge of the parallel shear spectrum is the starting point to understand the shear instability within internal waves. In this chapter we review the spectral analysis of parallel stratified shear layers, and present some original results not covered (at the best of our knowledge) by the current literature.

2.1 The Taylor–Goldstein equation

Consider a stratified inviscid parallel shear layer, defined by the (non-dimensional) velocity profile $U(y) = (U(y), 0)$ and the density profile $R(y) = 1 + \sigma r(y)$, where $\sigma \ll 1$, such that the Boussinesq approximation applies, and $R_y < 0$ for static stability. For ease of comparison with the familiar results by [45], here we non-dimensionalize upon the shear maximum velocity $V$, and the shear layer thickness $\ell$. We choose the same thickness for both shear and stratification, keeping in mind the conditions typical of internal waves, where the density and shear profiles are functionally related and cannot be set independently. In such a way we can fix $U_y(0) = 1$ and $r_y(0) = -1$ (assuming without loss of generality that $U_y$ is maximum at 0). The relative importance of shear and stratification is measured by the local Richardson number $\text{Ri}$,

$$\text{Ri} \equiv -g \frac{1}{R} \frac{dR}{dy} \left/ \left( \frac{dU}{dy} \right)^2 \right.. \quad (2.1)$$
As a single representative value it is customary to use the overall Richardson number $J \equiv \text{Ri}(0)$.

It is well known that the two-dimensional spectral linear stability, i.e. the evolution of small perturbations in the form

$$\hat{\psi}(x, y, t) = \hat{\psi}(y)e^{i(kx-ct)} + \text{c.c.}, \quad (2.2)$$

where $\psi$ is the perturbation of the streamfunction, and $c = c_R + ic_I$ is the complex phase speed, is governed by the Taylor–Goldstein eigenvalue problem in the form (under the Boussinesq approximation)

$$\hat{\psi}_{yy} + \left[ \frac{J\beta_y}{(U-c)^2} - \frac{U_{yy}}{U-c} - k^2 \right] \hat{\psi} = 0, \quad (2.3)$$

where $\beta = -r(y)$. In what follows we shall consider a free shear layer, and apply the boundary conditions $|\hat{\psi}| \to 0$ as $y \to \pm\infty$.

The study of the spectrum of the operator 2.3, like other stability operators (e.g., Rayleigh, Orr–Sommerfeld) can be done following two specular approaches, each one leading to a different paradigm of stability: temporal and spatial. In the temporal viewpoint the wavenumber $k$ is given and real, while the phase speed $c$ (or the frequency $\omega$) is the unknown, possibly complex, eigenvalue. According to the spatial viewpoint (see, e.g., the monography by Schmid & Henningson [83]), the wavenumber $k$ is regarded as the (unknown) eigenvalue in the Taylor–Goldstein equation while the frequency $\omega$ is real and fixed. The occurrence of a negative imaginary part of $k$, $k = k_R + ik_I$ with $k_I < 0$, would correspond to the spatial growth of plane waves $\hat{\psi}(y)e^{i(kx-\omega t)}$ in the direction of increasing $x$. The spatial formulation arises naturally in the so-called signalling problem (see, e.g., [43]), when spatial instability can be viewed as the result of an upstream periodic source of excitation.
2.1.1 Discrete spectrum

The temporal spectrum of the Taylor–Goldstein equation has been the subject of extensive studies since the 1960’s. Most notably are the seminal works by J.W. Miles and L.N. Howard [73, 74, 48, 50]. Equation (2.3) has a regular singularity at $U(y_c) = c$, hence two fundamental solutions have algebraic branch points of index

$$\hat{\psi} \sim (y - y_c)^{\frac{1}{2} \pm \nu}, \quad \text{as} \quad y \to y_c,$$

where $\nu = \left(\frac{1}{4} - \text{Ri}(y_c)\right)^{1/2}$ is obtained from Frobenius analysis.

The birth of an instability pocket for a wave-induced shear flow corresponds to the birth of an imaginary part $c_I$ for an eigenvalue of the linear problem (2.3). Under suitable assumptions on the known coefficients in this equation, the eigenvalues can be regarded as analytic functions of $J$ and $k$. The process of creation of an imaginary spectral component is best illustrated in the context of a specific example. A choice which is convenient for comparison with well established results in the literature (e.g., [45]) is

$$U(y) = \tanh(y), \quad \beta(y) = -\tanh(y).$$

(2.4)

This will also be the form used in the numerical simulation of internal waves later on in §4.2. In this case it can be shown that there exists a single neutral curve (given by $J(k) = k(1 - k)$), defined as the curve in the parameter plane $(J, k)$ separating real (stable) from complex (unstable) spectrum, on which the imaginary component of the complex spectrum vanishes. For the shear (2.4) it can be shown that the unstable mode exists and is unique inside the instability region.

Previous studies [74, 49] have discussed by local analysis the character of $c$ regarded as an analytic function of $J$ and $k$ in the neighborhood of the neutral curve. A main point of their analysis for this case is to show that $c_I = 0$ occurs only with $c_I$ changing
Figure 2.1: Deformation of the integration contour for computing eigenfunctions of (2.3) in the complexified $y$-plane as the branch point $y_c$ crosses the real axis, going from unstable (left panel) to stable (right panel).

Sign across the neutral curve, to conclude that singular neutral modes can exist only on a stability boundary. However, since to any complex stable eigenvalue ($c_I < 0$) always corresponds an unstable one $c_I > 0$ (by the complex conjugate symmetry of equation (2.3)), the results of Miles and Howard seem to lead to the conclusion that an unstable mode always exists beyond the neutral curve. (Such apparently unresolved inconsistency is remarked upon Yih’s monograph [103], p. 272.) In order to show how the eigenvalues can indeed be continued beyond the neutral curve (consistently with Miles and Howard analysis) we solve the Taylor–Goldstein problem in the $y$ complex plane, ignoring the physical requirement to have continuous eigenfunctions defined only for real $y$. We apply a shooting method (see, e.g., Hazel, ib.), however we do so for a path of integration deformed away from the real axis, oriented to loop around the branch point, see figure 8.3.

The unstable eigenvalue branch is reported in figures 2.2a and 2.2b, for the real and imaginary parts of $c$ respectively, with $k = 0.5$. When the unstable branch becomes stable ($J = 1/4$) $y_c$ reaches the real axis, and the eigenvalue cannot be tracked any further unless we switch integration path from $\mathcal{R}$ to $\mathcal{C}^+$. The second path allows to access the stable continuation of the unstable branch (dashed in the figure), however the associated eigenfunctions are unphysical because the branch-cut crosses the real
Figure 2.2: Spectrum calculations for $k = 0.5$. (a) $c_R$ for the unstable mode; (b) $c_I$; (c) real $c$ for a few neutral modes. All eigenvalues are plotted against the overall Richardson number. (d) locus in the complex plane of the branch point $y_c$ corresponding to the unstable eigenvalue as $J$ is varied. The lines are dashed after the branch point crosses the real axis (unphysical modes).

line giving rise to discontinuous eigenfunctions. (The same holds for the conjugate mode, i.e., the stable complex branch can be continued as an unstable but unphysical branch my deforming the path to $C^-$ as shown in figure 2.2b). We complete the spectral picture by also showing, in figure 2.2c, the first few real eigenvalues belonging to the neutral-mode branches. We emphasize the collapse of this part of the spectrum on the extrema of $U(y)$ as $J \to 0$ ($U_{1,2} = \pm 1$). This as well as other main features of the Taylor–Goldstein spectrum, reviewed in this section for a localized monotonic parallel shear profile, will be reconsidered in the context of wave-induced shears next.
2.1.2 Continuous spectrum

In the previous section we have seen that for fixed real $k$, the Taylor–Goldstein equation possesses a discrete set of stable eigenvalues, and, if $\text{Ri} < 1/4$, also a discrete set of unstable (complex) eigenvalues (typically a single one). Furthermore, there exists a continuous set of eigenvalues $c \in [U_{\text{min}}, U_{\text{max}}]$, referred to as the continuous spectrum [26] [8]). The associated eigenfunctions, $\hat{\phi}(y, c)$, must be properly accounted for in order to obtain a complete basis of eigenmodes for solving initial value problems. In what follows we shall discuss particular solutions constructed using only eigenfunctions associated with the continuous spectrum.

To obtain such eigenfunctions it is necessary to weaken the conditions under which the discrete-spectrum eigenfunctions are sought. For instance, the Orr–Sommerfeld equation in unbounded domains has a continuous spectrum which is found once the eigenfunctions are required to be bounded, as opposed to decaying (see Grosch & Salwen [44]). In contrast, here we seek weak solutions of the Taylor–Goldstein equation by fixing $c$ as specified above, enforcing the same boundary conditions as for the discrete-spectrum modes, but allowing for a branch-point singularity on the real $y$-axis at $y = y_c(c)$.

Despite the fact that the formal theory of generalized eigenfunctions $\hat{\phi}(y, c)$ is rather technical [37] their practical construction is rather easy to envisage. Such construction consists in patching regular solutions of the Taylor–Goldstein equation across the critical point $y_c$. The solutions on either side of the singularity must satisfy the boundary condition at the respective boundary. Such solutions are analytic in both arguments $y$ and $c$, with a branch-cut singularity at $y = y_c$, and, correspondingly, at $c = U(y)$. Just like the discrete-spectrum eigenfunctions, the $\hat{\phi}$'s can be expressed by Frobenius
expansions in either $y$ or $c$. The $y$-expansion is given by

$$
\phi(y, c) = (y - y_c)^{1/2+\nu} \sum_{n=0}^{+\infty} a_n (y - y_c)^n + (y - y_c)^{1/2-\nu} \sum_{n=0}^{+\infty} b_n (y - y_c)^n,
$$

(2.5)

where

$$
\nu(c) = \left( \frac{1}{4} - \text{Ri}(y_c(c)) \right)^{1/2}.
$$

The $c$-expansion has the same structure, i.e., it is obtained by replacing $y - y_c(c)$ with $c - U(y)$, and the same indicial exponent now regarded as a function of $y$, $\nu = \nu(y) = \left( \frac{1}{4} - \text{Ri}(y) \right)^{1/2}$. This can be verified by using such expansion inside (2.3). As an alternative, one can fix $\omega = ck$ and regard $k$ as a free parameter. Also in this case, with $\phi = \phi(y, k)$, Frobenius expansions in either $(y - y_c(k))$ or $(k - k_c(y))$ hold, with $\nu = \nu(k)$ or $\nu = \nu(y)$ respectively.

It must be noticed that, unlike the discrete spectrum, the expansion (2.5) is one-sided, i.e., it holds only on one side of the point $y = y_c$ on the real axis. Indeed, due to the lack of a continuation rule we are free to patch in an arbitrary way the left- and right-side solution of the Taylor–Goldstein equation (2.3) with $c = U(y_c)$ to obtain a continuous function $\hat{\phi}(y, c)$. This implies that for any $c$ in the continuous spectrum there is a pair of eigenfunctions $\left( \hat{\phi}^+, \hat{\phi}^- \right)$. Without loss of generality we set

$$
\begin{cases}
\hat{\phi}^+(y, c) = 0 & \text{for } y < y_c, \\
\hat{\phi}^-(y, c) = 0 & \text{for } y > y_c.
\end{cases}
$$

In figure 2.3 a few eigenfunctions, from both the continuous and the discrete spectrum are shown. Observe that the discrete-spectrum modes are near identical to each other around the core of the shear ($y = 0$), and their support is mostly localized on the peripheral part of the shear. This fact suggests the importance of the continuous spectrum modes in capturing the dynamics occurring in the shear core. In figure 2.4
an unstable discrete-spectrum eigenfunction is shown.

Figure 2.3: Eigenfunctions computed on the tanh shear layer in a bounded domain, all computed for $k = 1$. The overall Richardson number is $J = 0.35$ (no complex spectrum). Rigid-lid boundary conditions are applied at the domain boundaries $y = \pm 6$. Left plot: three pairs of continuous spectrum modes, $\hat{\phi}^+$ (solid lines) and $\hat{\phi}^-$ (dashed lines). Right plot: first three pairs of discrete spectrum modes, $\hat{\psi}_n$, corresponding to the three largest eigenvalues $c_n > U_{\text{max}}$ (solid lines) and the three smallest $c_n < U_{\text{min}}$ (dashed lines).

Figure 2.4: Real and imaginary parts of the unstable mode eigenfunction. Computed on the tanh shear layer in a bounded domain, for $k = 0.5$ and $J = 0.1$. Rigid-lid boundary conditions are applied at the domain boundaries $y = \pm 6$. 

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3.1 Model for the internal wave structure

In this chapter we connect the spectral analysis presented in chapter 2 to the case of wave-induced shear layers. It is largely convenient for the purpose of computations to employ a simplified fully-analytic model for an internal wave in a continuous stratification. The model is essentially a combination of the two-layer strongly non linear model (introduced in §1.4.2) with a correction applied around the interface. Used as an approximation to the reference background flow for the stability analysis, the model allows to compute the local shear eigenvalues efficiently, by finding the zeros of functions computed explicitly.

3.1.1 Three-layer configuration

Consider the case of a stratified (incompressible Euler) fluid whose rest configuration consists of two constant-density layers, with \( \rho = \rho_1 \) and \( \rho = \rho_2 \) respectively for the upper and lower layer, and a linearly-stratified layer sandwiched between them,

\[
\rho(\psi) = \rho_2 + \frac{\rho_1 - \rho_2}{h_M} \left( \frac{\psi}{c_W} - h_2 \right), \quad \text{for} \quad h_2 < \frac{\psi}{c_W} < h_2 + h_M.
\] (3.1)
Such setup is typically used in the modeling of oceanic internal waves, see, e.g., [41]. Solitary-wave solutions supported by such stratification have the structure sketched in Fig. 8.3. Diffusion of the stratifying agent can be neglected on the time scale of wave propagation, so that the fluid domain $\mathcal{D}$ can be partitioned in two regions $\mathcal{D}_1$ (upper) and $\mathcal{D}_2$ (lower), and an intermediate region $\mathcal{D}_M$ in which density varies between $\rho_1$ and $\rho_2$ (i.e., the pycnocline). Let the interfaces between $\mathcal{D}_i$ and $\mathcal{D}_M$ be denoted by $\zeta_i(x)$, $i = 1, 2$, and let $\zeta(x)$ be the intermediate streamline on which $\rho = (\rho_1 + \rho_2)/2$.

The DJL equation reduces to the Laplace equation inside $\mathcal{D}_1$ and $\mathcal{D}_2$, and the Helmholtz equation inside $\mathcal{D}_M$:

$$\nabla^2 \psi_i = 0 \quad \text{in} \quad \mathcal{D}_i, \quad (i = 1, 2) \quad (3.2)$$

$$\nabla^2 \psi_M + \frac{N^2}{c_W^2} (\psi_M - c_W h(x)) = 0 \quad \text{in} \quad \mathcal{D}_M, \quad (3.3)$$

where the function $h(x)$, the height of a point in the fluid domain, is introduced for later convenience, and $N^2 \equiv -g\rho_y$ is the square of the so-called Brunt–Väisälä frequency. On internal boundaries the continuity of tangential velocity and pressure must be enforced

$$\Delta(u \cdot n) = 0, \quad \Delta p = 0, \quad (3.4)$$

where $n$ is the unit vector normal to the interface, and $\Delta$ denotes the jump of a
quantity across an interface. In terms of the streamfunction, all boundary and interface conditions are

\[ \psi_1 = c_W \ell, \quad \psi_2 = 0, \quad \text{at} \quad y = \ell \quad \text{and} \quad y = 0, \]  
\[ \psi_i = \psi_M = c_W \zeta_i \infty, \quad \text{at} \quad y = \zeta_i, \]  
\[ \partial_n \psi_i = \partial_n \psi_M, \quad \text{at} \quad y = \zeta_i \quad (i = 1, 2), \]  

where \( \partial_n \) is the derivative in the direction of \( \mathbf{n} \). We recall that (3.5) is the slip-wall condition, (3.6) expresses the kinematic condition at the interface and (3.7) derives from the continuity of pressure. The label “\( \infty \)” denotes the far-field value of a variable, thus \( \zeta_{1 \infty} = 1 - h_1, \zeta_{2 \infty} = h_2, \zeta_{\infty} = h_2 + h_M / 2 \).

In what follows we report the expressions for the wave field. Despite its simplicity, this is an asymptotically valid approximant in the joint limit of long waves/thin pycnoclines, for basic stratifications \( \bar{\rho}(y) \) consisting of two homogeneous layers with a linear pycnocline in between. The parameters defining the unperturbed stratification are the two limiting densities \( \rho_2 \) and \( \rho_1 \), the pycnocline thickness \( \delta \), and the vertical location \( y = h_2 \) of its mid point, see figure 3.2 for a sketch. The horizontal velocity generated by the wave, which is substantially larger than the vertical component, is given by the model as

\[ U = \begin{cases} 
U_1 & \zeta_1 < y < 1, \\
U_2 + (y - \zeta_2)(U_1 - U_2)/\delta_p & \zeta_2 \leq y \leq \zeta_1, \\
U_2 & 0 < y < \zeta_2,
\end{cases} \]  

where \( U_j \) and \( \zeta_j \ (j = 1, 2) \) are functions of \( x \), and will be defined shortly. The density profile which is consistent with the specific functional relation \( R(\psi) \) holding in the case
Figure 3.2: Schematic of the 3-layers model.

The local pycnocline thickness, $\delta_p = \delta_p(x)$, is determined by imposing conservation of volumetric flux

$$\delta_p \equiv \zeta_1 - \zeta_2 = \frac{2\delta c_W}{U_1 + U_2},$$

(3.10)

while the internal interfaces $\zeta_j$ are determined by the condition $R(\zeta) = (\rho_1 + \rho_2)/2$, which yields

$$\zeta_2 = \zeta - \frac{U_2 - \left(\frac{1}{2} U_1^2 + \frac{1}{2} U_2^2\right)^{1/2}}{U_2 - U_1} \delta_p,$$

and

$$\zeta_1 = \zeta_2 + \delta_p,$$

for waves of depression.

The central mean-density interface $\zeta$ is provided by the strongly nonlinear model for internal waves in a two-layer system described in §1.4.2. Following [29] such interface is obtained by first setting the wave speed $c_W$, and then solving a differential equation.
in the form
\[ \zeta_x = F(\zeta, c_W, \rho_1, \rho_2, h_1, h_2), \]
where, \( h_1 \) and \( h_2 \) are the (effective) thicknesses of the upper and lower layer respectively (see Camassa & Tiron, 2011, for a criterion on how to choose optimal two-layer parameters). A solitary wave solution of such equation exists provided \( c_W \) is not greater than a maximum attainable value (function of the remaining parameters). An analytic expression involving elliptic functions (see Choi & Camassa, 1999) is available. The upper- and lower-layer flow speeds are respectively given by
\[ U_1 = c_W h_1 / (h_1 - \zeta), \quad U_2 = c_W h_2 / (h_2 - \zeta). \] (3.11)

### 3.2 Computation of the local spectrum

We use the above model to compute the local eigenvalues of the shear layer. The shear that results from setting \( x \) as a fixed parameter in (3.8) and (3.9) is linear in the velocity and parabolic in the density inside the pycnocline, and represents the parallel flow that will be considered in the rest of this section.

For piecewise-smooth profiles we have to find solutions of the Taylor–Goldstein equation (2.3) in each layer, and then enforce continuity of vertical displacement and pressure at the internal interfaces. Let \( \eta = \eta(x, y, t) \) be the vertical displacements of isopycnals from the unperturbed steady state, and \( p \) the perturbation pressure. Like the other perturbation variables, these are sought in the form \( \eta = \hat{\eta} \exp [ik(x - ct)] + c.c. \) and \( p = \hat{p} \exp [ik(x - ct)] + c.c. \). Using the linearized equations of motion we can express \( \hat{\eta} \) and \( \hat{p} \) in terms of the perturbation streamfunction:
\[ \hat{\eta} = \hat{\psi} / (U - c), \]
\[ \hat{p} = (U - c)\hat{\psi}_y + U_y \hat{\psi}. \]

By imposing the continuity of such quantities we obtain the interface conditions

\[ \Delta_j \hat{\psi} = 0, \]
\[ \Delta_j[(U - c)\hat{\psi}_y + U_y \hat{\psi}] = 0, \]

for \( j = 1, 2 \), where \( \Delta_j \) denotes the jump of a quantity across \( \zeta_j \).

In the upper and lower layers, we retain only the decaying solution of (2.3), as in a free shear layer, which is an acceptable approximation in the case of thin pycnoclines. We then have to construct an eigenmode by using the four fundamental solutions

\[
\hat{\psi}(y) = \begin{cases} 
A\hat{\phi}_{1U} & \zeta_1 < y < 1, \\
B\hat{\phi}_{1M} + C\hat{\phi}_{2M} & \zeta_2 \leq y \leq \zeta_1, \\
D\hat{\phi}_{2L} & 0 < y < \zeta_2,
\end{cases}
\]

where each function satisfies the Taylor–Goldstein equation in the respective layer, and \( A, B, C, D \) are constants to be determined. For \( y > \zeta_1 \) and \( y < \zeta_2 \) it is easily seen that \( \beta = U_{yy} = 0 \), hence the Taylor–Goldstein equation simplifies to \( \hat{\psi}_{yy} - k^2 \hat{\psi} = 0 \), and

\[
\hat{\phi}_{1U} = e^{-k^2(y-\zeta_1)}, \\
\hat{\phi}_{2L} = e^{k^2(y-\zeta_2)}. 
\]

In the intermediate layer (\( \zeta_2 < y < \zeta_1 \)) the change of independent variable

\[
z = \frac{2k}{U_y}[U_2 + U_y(y - \zeta_2) - c],
\]

maps the Taylor-Goldstein equation (2.3) with \( U(y) \) and \( \beta(y) \) given respectively by
(3.8) and (3.9), with $J = g\sigma\delta/c_W$, into the Whittaker’s hypergeometric equation

$$\hat{\psi}_{zz} + \left(\frac{1}{4} - \mu^2 + \kappa \frac{1}{z} - \frac{1}{4}\right) \hat{\psi} = 0,$$

(3.14)

where

$$\kappa = n + \mu + \frac{1}{2}, \quad n = \frac{J(\rho_1 - \rho_2)}{\rho_0 k(U_1^2 - U_2^2)} - \mu - \frac{1}{2}, \quad \mu^2 = -Jc \frac{\rho_1 - \rho_2}{\rho_0 U_0^2 c_W \delta} + \frac{1}{4}.$$

Here $\rho_0$ is the reference density of the Boussinesq approximation.

The fundamental solutions of (3.14) are the so-called Whittaker’s functions $M_{\kappa,\mu}(z)$ and $W_{\kappa,\mu}(z)$ (following Abramowitz & Stegun 1964), hence

$$\hat{\phi}_{1M}(y, c) = M_{\kappa(c),\mu(c)}(z(y, c)),$$
$$\hat{\phi}_{2M}(y, c) = W_{\kappa(c),\mu(c)}(z(y, c)).$$

Note that Whittaker’s functions have an algebraic branch-cut emanating from the origin in the $z$-plane. We then have to interpret such functions as the branches which are continuous over the line segment connecting $z(y_L)$ and $z(y_U)$.

The interface conditions (3.12) and (3.13) yield a homogeneous $4 \times 4$ linear system in the unknown coefficients $A$, $B$, $C$, and $D$. The eigenvalue $c$ is determined by setting the corresponding determinant equal zero to enforce solvability. However, it is possible to reduce the problem size down to $2 \times 2$ by solving first the two equations (3.12) for $A$ and $D$. Standard manipulations give

$$\text{Det} \left[D(c, k; x)\right] = 0,$$

(3.15)
with

\[
D \equiv \begin{bmatrix}
\hat{\phi}_{1M} + \left( k - \frac{U_y}{U - c} \right) \hat{\phi}_{1M} & \hat{\phi}_{2M} + \left( k - \frac{U_y}{U - c} \right) \hat{\phi}_{2M} \\
\hat{\phi}_{1M} - \left( k + \frac{U_y}{U - c} \right) \hat{\phi}_{1M} & \hat{\phi}_{2M} - \left( k + \frac{U_y}{U - c} \right) \hat{\phi}_{2M}
\end{bmatrix},
\]  
\tag{3.16}

where in the first (second) row of the matrix \( D \) all functions are evaluated at \( y = \zeta_1 \) (\( y = \zeta_2 \)). Standard software packages that allow manipulation of special functions can be employed to easily find the roots of the above expression efficiently and to any prescribed accuracy.

Several eigenvalue branches have been computed in the way just described, and reported in figure 3.3 as a function of \( x \) along wave-induced shears. In figure 3.3a the parameters correspond to wave W1 (see the upcoming table 4.2), for \( k = k_B \) from runs W1R and W1L (W1R is the same used in the example of section 4.1.1). No unstable eigenvalue is detected in this case. On the other hand figures 3.3b and 3.3c correspond to a wave with thinner pycnocline, case W2, which yields local instability about the wave’s maximum reported (panel (c)) as the growth rate \( \omega_I \) vs. \( x \). Away from the wave center the eigenvalues approach the baroclinic-mode limit. For linear stratification and \( U \equiv 0 \), the formula (3.15) reduces into the much simpler form

\[
\theta \sin \left( \frac{\theta \delta}{2} \right) - k \cos \left( \frac{\theta \delta}{2} \right) = 0, \quad \text{or} \quad \theta \cos \left( \frac{\theta \delta}{2} \right) + k \sin \left( \frac{\theta \delta}{2} \right) = 0,
\]

for symmetric \( (n = 0, 2, 4, \ldots) \) and antisymmetric modes \( (n = 1, 3, \ldots) \) respectively, where \( \theta^2 = -g(\rho_1 - \rho_2)/(\rho_0 \delta c^2) - k^2 \). Such limiting values of the \( c_n \)'s are included in figure 3.3 for reference.

The qualitative features of these results, in particular the eigenvalue clustering and the unstable bifurcation traversing the neutral curve, are not affected by the specific pycnocline structure assumed. This behaviour is analogous to the one relative to the
Figure 3.3: Local eigenvalues computed on the background flow model as a function of $x - x_c$, with $x_c = 8$. (a) Phase speed $c_R$ for the W1 wave, with $k = k_B$ for run W1R (or equivalently W1L). The branches continuing the first 6 baroclinic modes are shown. Grey-thick curves are the velocity extrema $U_1$ and $U_2$ from the model (recall $U_2 > U_1$). (b) Similar plot for wave W2 (thinner pycnocline), with $k = k_B$ for run W2L1 (or equivalently W2R1). An unstable mode develops near $x = x_0$. (c) Growth rate $\omega_I = kc_I$ for the unstable mode. (d) Wave profile represented by $\zeta(x)$. The $|x| \to \infty$ limiting values for $c_R$ are reported in (a) and (b) (dashed lines).
Figure 3.4: Horizontal velocity (a)–(c) and density (b)–(d) profiles at the wave’s maximum reconstructed from the model (dashed lines) versus the full numerical computations (solid lines). Pycnocline thickness $\delta = 0.1$ (a)–(b) and $\delta = 0.05$ (c)–(d).

hyperbolic-tangent profiles reported in figures 2.2a and 2.2b, where $J$ plays a role analogous to $x$ by setting the relative strength of shear and stratification.

The model is capable of capturing realistic details. For instance the phase speed of the unstable mode, figure 3.3c, is slightly lower than $c_w$, consistently with the observation reported by [40] from lab experiments that unstable billows travel at a speed $\approx 0.1c_w$ when observed in the lab frame.

Another major feature of the spectrum is the strong clustering of the neutral-mode eigenvalues which is present for both background waves $W_1$ and $W_2$. Such clustering can be shown to be a general feature of the real spectrum for a wide class of shear flows. For instance, by switching the roles of $c$ and $k$, i.e., by considering $c$ as a real parameter in the complement of the velocity range interval $c \in [U_1, U_2]^{c}$ and searching for eigenvalues $k^2$, the Taylor-Goldstein eigenvalue problem (2.3) becomes a standard potential-well Schrödinger problem, with the minimum of the potential decreasing to
Figure 3.5: Eigenvalues computed from the model (circles) versus the computations based on the actual profiles (diamonds) from the DJL numerical solution. The real eigenvalues correspond to the first and second neutral mode of the family approaching $U_1^+$ at the wave maximum, for $\delta = 0.1$, the complex ones are the unstable mode for $\delta = 0.05$.

$-\infty$ as $c$ approaches from outside the interval $[U_1, U_2]$. This assures that a countable number of eigenvalue curves $k_n^2(c)$ in the appropriate $(c,k)$-quadrants approach their vertical asymptotes at $c = U_1$ and $c = U_2$, thereby guaranteeing the existence of a clustering spectrum $c_n^{(1)} \to U_1^-$ and $c_n^{(2)} \to U_2^+$ for fixed $k^2 > 0$.

Notice that the neutral-mode branches approach, but do not intersect, the curves given by the upper- and lower-layer velocities as we move near the wave maximum. This is supported by careful numerical computations by arithmetics of increasing precision. Numerical root finding eventually fails as $c$ approaches $U_1$ or $U_2$, due to the Taylor-Goldstein equation becoming close to singular, however high-precision arithmetics allows tracking of the eigenvalues well beyond points depicted in figure 3.3, which we stress should not be viewed as terminal points of the neutral branches.

In figures 3.4a–3.4d we offer a comparison between the profiles derived form the model wave field (3.8)–(3.9) and the full computations performed with the TEW algorithm. In both cases the wave amplitude is close to its maximum, and the pycnocline displacement is closely matched. The propagation speed is $c_W = 0.2081$ and
\( c_W = 0.2127 \) respectively for the TEW computation and the model. In general, when using the two-layer model to approximate a continuously-stratified wave, it is convenient to match the wave amplitude rather than the propagation speed, as \( c_W \) is weakly sensitive to the amplitude. This level of accuracy is satisfactory for the purpose of the present study, see [16] for more details, and [23] for a discussion of improvements in applications of the strongly nonlinear model.

The accuracy of the eigenvalues computed on the model wave-flow, with respect to those computed by shooting-method on the shear and density profiles of the full numerical solution of the DJL equation, is illustrated by figure 3.5. The agreement is reasonable, especially in view of the simple leading order nature of the model. For instance, at the wave maximum, the phase speed of the first neutral mode is \( c = 0.3445 \) and \( c = 0.3563 \), respectively by using equation (3.15) or the full computation.

The complete characterization of the spectral properties presented in this section refers to the same waves that are used as backgrounds in the next section, and will aid in the interpretation of the numerical results thereof.
Chapter 4

RESPONSE OF LARGE AMPLITUDE INTERNAL WAVES TO
UPSTREAM PERTURBATIONS

In this chapter a series of numerical experiments is presented and discussed in order
to assess the relation existing between the local spectrum along a wave profile (discussed
in chapter 3) and the evolution of prescribed perturbations. No explicit verification of
such relation seems to have been reported by far, despite the fact that in previous
studies of internal waves instability (see references in §1.2) much reasoning is based on
the local spectrum.

Our setup consists of an initial value problem in which a small-amplitude long wave-
packet is superimposed on a pre-computed basic flow consisting of a solitary-wave
solution of the stratified, incompressible Euler equations. Such a setup corresponds
to the physically relevant case of a perturbation upstream of an approaching (large
amplitude) solitary wave. We focus on how the perturbation evolves throughout the
shear region that the solitary wave produces during its propagation. In particular, we
shall see that the internal wave can act as a suppressor of the perturbation, absorbing
its energy and leaving a quieter state in its wake. This setup is similar to a transmission
problem, with the internal wave flow acting as a “black box” absorbing a prescribed
input signal released upstream and shedding it downstream. Direct observation of such
processes seems to be novel in the case of internal waves, in particular of how the wave-
induced shear responds to the parameters of the upstream (baroclinic) modes whose
superposition carries a given disturbance.

The internal mechanisms of the “black box” can be effectively illustrated when the upstream perturbation is chosen as a single baroclinic mode of the undisturbed (quiescent state) stratification. The evolution of such perturbations through the wave-induced shear then isolates two fundamental dynamical features that appear not to have received much attention so far: (i) the non-normal evolution of the perturbation due to eigenmodes being non-orthogonal in the presence of shear, and (ii) the interplay of non-normality with the non-parallel spatial dependence of the background flow. These two features are unrelated to linear instability of the stratified shear flow.

Depending on the parameters of the equilibrium state and the wave amplitude, the self-induced shear region may also include an “instability pocket,” i.e., the portion of the fluid domain where the local Richardson number (Ri) falls below $1/4$ (according to the well known criterion of Miles 1961, and Howard 1961, for parallel stratified shears). Thus, we also consider a third “black box” mechanism that can alter the input signal by upstream perturbations provided by the possibility of shear instabilities. In such cases, the entrained perturbation can in turn feed the unstable modes present in unstable pockets, and, depending on its amplitude, lead to the development of Kelvin–Helmholtz roll-ups within the pocket. The process is reversed at the downstream side of the pocket, thereby determining the resulting form of the original perturbation in the internal wave’s wake.

4.1 Problem setup

4.1.1 Single baroclinic mode disturbance of internal solitary waves propagation

We compute a large-amplitude solitary wave solution of the DJL equation using a code based on the algorithm of [99] (hereafter referred to as TEW). To determine a
particular solitary wave we set the unperturbed stratification

$$\bar{\rho} = \frac{\rho_2 + \rho_1}{2} + \frac{\rho_1 - \rho_2}{2} \tanh[(y - y_0)/\delta].$$  \hspace{1cm} (4.1)

and select the wave amplitude. (The Boussinesq approximation would require $\rho_2 - \rho_1 \ll \rho_{1,2}$, a condition verified in salt-stratified lab experiments as well as in field conditions.)

For the equilibrium density (4.1) with sufficiently sharp pycnoclines $\delta \ll y_0$, the amplitude of nonlinear solitary waves (measurable, e.g., by isopycnal displacement from equilibrium) is known to have a limiting value (see, e.g., Lamb & Wan [58]) where the wave flattens and tends to the limit of a propagating front (i.e., a ‘conjugate state’). In this work we will simply refer to the $x$-position of the maximum isopycnal displacement as the wave maximum, and its $y$-position as the wave amplitude. We will be mostly concerned with waves whose amplitude is close to the limiting value. The velocity and density fields of such background travelling wave solution in the wave reference frame are denoted by $U(x)$ and $R(x)$ respectively. In an ideal unbounded domain one would have $R \to \bar{\rho}$ and $U \to (c_W, 0)$ as $|x| \to \infty$. This is approximately true for our numerical implementation, as the horizontal extent of the domain is large (cf. Section 4.2 for details.) We denote the extrema of the horizontal velocity component in the wave self-induced shear $U$ by $U_2(x)$ and $U_1(x)$, respectively, with $U_2(x) > c_W > U_1(x)$ in the wave frame.

Fluctuations with respect to the basic solution will be denoted by $u'$ and $\rho'$,

$$u = U + u', \quad \rho = R + \rho',$$ \hspace{1cm} (4.2)

and similarly for any other variable.

In the absence of shear ($U = 0$) and in the lab frame (where the fluid is at rest at infinity), the unperturbed stratification reduces to $R = \bar{\rho}$ and supports neutrally-stable
linear baroclinic modes, governed by the eigenvalue problem

\[
\hat{\psi}_{yy} + \left( g\bar{\rho}_y / (\bar{\rho}c^2) - k^2 \right) \hat{\psi} = 0 \tag{4.3}
\]

for the sinusoidal perturbation streamfunction \( \psi' = e^{i(kx-\omega t)} \hat{\psi}(y,k) \), with phase speed \( c(k) \equiv \omega / k \), supplemented by the slip-wall boundary conditions \( \hat{\psi}(0) = \hat{\psi}(1) = 0 \). For \( \bar{\rho} \) given by (4.1), and assuming the Boussinesq approximation, whereby

\[
\frac{\bar{\rho}_y}{\bar{\rho}} \sim \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1} \frac{\text{sech}^2[(y - y_0)/\delta]}{\delta},
\]

eigenvalues \( c \) form a countable sequence, which for thin pycnoclines \( \delta \ll 1 \) can be shown (see, e.g., Banks et al. 1976) to be approximated by

\[
c_n^2 = g \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1} \frac{4\delta}{(1 + 2n + 2\delta k)^2 - 1}; \quad n = 0, 1, \ldots,
\]

for any fixed wavenumber \( k \). Such modes give rise to a system of waves occurring in pairs with the same phase speed \( |c| \) but opposite direction of propagation. Thus, eigenvalue pairs can be ordered in a sequence \( |c_1| > |c_2| > \cdots > 0 \) accumulating onto zero, i.e., \( c_n \to 0 \) as \( n \to \infty \). This remains true for more general density backgrounds, as one can show by writing the eigenvalue problem in nonlocal symmetric form, whence the above property, as well as others (like completeness of eigenfunctions), follow from the classical spectral theory of integral operators (see, e.g., [97]).

In the upstream region we superimpose a small perturbation based on the first baroclinic mode of the undisturbed stratification for a wavenumber \( k = k_B \):

\[
\begin{pmatrix}
\psi' (x, y) \\
\rho' (x, y)
\end{pmatrix}
= \begin{pmatrix}
\hat{\psi}(y, k_B) \\
\hat{\rho}(y, k_B)
\end{pmatrix}
a \cos(k_Bx) \exp \left[-(x - x_0)^2/\Delta x\right] \quad \text{at} \quad t = 0. \tag{4.4}
\]
Figure 4.1: Simulation of an internal wave interacting with a train of upstream perturbing mode-1 baroclinic waves. The horizontal velocity component of the perturbation is depicted, internal labels denote the time instants. This is case W1R in table 4.1, full discussion in §4.2. Labels correspond to time, and the pycnocline is referenced by two isolines ($R = 1.005, 1.015$) of the basic state density (varying in the range $1 \leq R \leq 1.02$). The domain shown is full-extent in the vertical, but only a center subsection of the domain is shown in the horizontal. The area inside the box is magnified in figure 4.5.

Notice that since the baroclinic modes are a complete basis any upstream disturbance can be reconstructed by their superposition. Also, notice that in the wave frame all perturbations travel to the right, as the speed of the background wave is larger than the speed of the linear modes.

Figure 4.1 depicts an example of a numerical simulation based on the setup we have described. The parameters we consider for this and other numerical simulations are reported in table 4.2. The snapshots show the perturbation entering the wave and being swept away by the internal shear layer. In this case the pycnocline thickness is not small enough to achieve $R_i < 1/4$, and no growth appears. Even though instability could be introduced by simply decreasing $\delta$, we choose its value in order to stay slightly away from instability and emphasize the perturbation dynamics. As one can see, the structure of
the perturbation changes substantially as it starts to experience the background shear. The full discussion of this and similar phenomena encountered during the perturbation evolution is the focus of the rest of the paper. In particular, the numerical simulations are the subject of §4.2. We now turn our attention to the details of the spectral stability and modal analysis of stratified shear flows next, beginning with the simplest case of parallel flows.

4.2 Numerical simulations

In the previous sections the spectrum of stratified shear layers and its spatial dependence along an internal wave has been investigated in some detail. We now present direct numerical simulations of the evolution of small perturbations within parallel and nonparallel wave-generated shear layers. The comparison of the two cases will focus on the developing physical structure of the perturbations as they enter the region upstream of the wave maximum. We will henceforth refer to this phase as the “entrainment” of the perturbation within the background shear. The quantitative analysis of this phase is carried out by using the energetic balances presented in §4.2.1.

The computations are performed using the VARDEN package, which solves the stratified Euler equations (for details see Almgren et al. 1998.) The boundary conditions are rigid slip-wall at the top and bottom, and periodic in the horizontal direction. The resolution is high compared to other numerical studies of stratified shear layer (e.g., Caulfield & Peltier 2000), since our focus is on the very fine structures that will be described later on in this section. For instance, in the parallel-shear simulations we use a square grid with 1024 points along the vertical with rigid lids located at 10δ distance from the center of the shear.

All the simulations presented here share the parameters \( \rho_1 = 1 \) and \( \rho_2 = 1.02 \), motivated by lab experimental values. The energy of the background travelling wave
Table 4.1: Parameters for the background flows used in the numerical simulations. All quantities are dimensional in SI units.

<table>
<thead>
<tr>
<th>Background</th>
<th>δ</th>
<th>c_W</th>
<th>R_{min}</th>
<th>L_x \times L_y</th>
<th>n_x \times n_y</th>
<th>\langle E_K(U) \rangle</th>
<th>\langle E_A(R, y) \rangle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel</td>
<td>0.05</td>
<td>–</td>
<td>0.49</td>
<td>\frac{4\pi}{10} \times \frac{32\pi}{10}</td>
<td>2048 \times 1024</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>W1</td>
<td>0.05</td>
<td>0.208</td>
<td>0.251</td>
<td>16 \times 1</td>
<td>16384 \times 1024</td>
<td>0.0382</td>
<td>0.0372</td>
</tr>
<tr>
<td>W2</td>
<td>0.03125</td>
<td>0.212</td>
<td>0.172</td>
<td>16 \times 1</td>
<td>16384 \times 1024</td>
<td>0.0381</td>
<td>0.0372</td>
</tr>
</tbody>
</table>

Table 4.2: Summary of runs performed with corresponding perturbation parameters. All quantities are dimensional in SI units.

<table>
<thead>
<tr>
<th>Perturbation</th>
<th>Runs</th>
<th>Background</th>
<th>k_B</th>
<th>c_W \pm c_0(k_B)</th>
<th>mode excited</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>Parallel</td>
<td>10</td>
<td>–</td>
<td>Right-going</td>
<td></td>
</tr>
<tr>
<td>W1L</td>
<td>W1</td>
<td>10</td>
<td>0.128</td>
<td>Left-going</td>
<td></td>
</tr>
<tr>
<td>W1R</td>
<td>W1</td>
<td>10</td>
<td>0.287</td>
<td>Right-going</td>
<td></td>
</tr>
<tr>
<td>W2L1</td>
<td>W2</td>
<td>16</td>
<td>0.149</td>
<td>Left-going</td>
<td></td>
</tr>
<tr>
<td>W2R1</td>
<td>W2</td>
<td>16</td>
<td>0.275</td>
<td>Right-going</td>
<td></td>
</tr>
<tr>
<td>W2L2</td>
<td>W2</td>
<td>26.24</td>
<td>0.167</td>
<td>Left-going</td>
<td></td>
</tr>
<tr>
<td>W2R2</td>
<td>W2</td>
<td>7.715</td>
<td>0.310</td>
<td>Right-going</td>
<td></td>
</tr>
</tbody>
</table>

solutions is chosen to be large enough to sample the transition from marginally stable to unstable self-induced local shears with minimal variations of the overall wave shapes. The wavenumber $k_B = 1/(2\delta)$ is chosen in order to fall in the most unstable range, when pockets of instability are present, according to the tanh-shear model of §2.1. The initial amplitude of the perturbations is small enough to be in the linear regime, and among the wave simulations we keep constant the maximum of the density perturbation. In this way we attain the same maximum isopycnal displacement relative to the pycnocline thickness (about 1% of $\delta$) at startup. All simulation parameters are summarized in table 4.2.
4.2.1 Energetic diagnostics

Before presenting the computational results, we introduce the energetic balances that we use to diagnose the flow evolution. As mentioned in §4.1, here we make use of perturbative analysis under the Boussinesq approximation, with $\rho_0 = 1$. The local kinetic and available potential energy (APE) densities are

$$E_K = \frac{|u|^2}{2}, \quad E_A = g \int_y^{Y(\rho)} [\bar{\rho}(s) - \rho] \, ds,$$

respectively (see, e.g., Lamb 2008 for a definition). In particular, $\bar{\rho}(y)$ is the minimal-potential-energy stratification obtainable by adiabatic rearrangement of the fluid particles, and $Y(\rho)$ is the height at which a fluid particle of density $\rho$ is found in such configuration. Often $E_A$ is preferred to the bare potential energy because it is pointwise positive-definite, and follows a simpler conservation law.

We introduce a decomposition of $E_K$ and $E_A$ into background and perturbative components. By recalling the flow decomposition (4.2) we Taylor-expand local energy densities about the basic flow up to first order, and denote remainders as $\mathcal{E}_K$ and $\mathcal{E}_A$:

$$E_K(U + u') = E_K(U) + \frac{\partial E_K}{\partial u_i}(U)u'_i + \mathcal{E}_K,$$

$$E_A(R + \rho', y) = E_A(R, y) + \frac{\partial E_A}{\partial \rho}(R, y)\rho' + \mathcal{E}_A. \quad (4.6)$$

The expressions for the second-order remainders are given by

$$\mathcal{E}_K = \frac{|u'|^2}{2}, \quad (4.8)$$

$$\mathcal{E}_A = g \int_{Y(R)}^{Y(R+\rho')}[\bar{\rho}(s) - R - \rho'] \, ds. \quad (4.9)$$

Observe that, just as $\mathcal{E}_K$, $\mathcal{E}_A$ is also positive definite as a consequence of $\bar{\rho}(y)$ being monotonic, and $\mathcal{E}_A$ is quadratic in $\rho'$ (for small $\rho'$). Therefore such quantity is suitable
to be regarded as the perturbation available potential energy.

Clearly, in absence of external forcing any perturbation-energy increase can only take place at the expense of the energy stored in the background flow. Therefore a closed energy balance can be obtained by including the variation of the background flow energy. The use of the first order terms inside (4.6), which we denote as

\[ e_K \equiv \frac{\partial E_K}{\partial u_i} (U) u'_i = U \cdot u' , \quad e_A \equiv \frac{\partial E_A}{\partial \rho} (R,y) \rho' = g \eta \rho' , \quad (4.10) \]

as opposed to the entire background energy variation, avoids the inconvenience of working with quantities possessing largely different orders of magnitude, as well as of dealing with the issue of infinite energy in unbounded domains. Also, in the above definitions \( \eta = y - Y(R) \) denotes the vertical displacement of density isolines of the background flow with respect to the \( \bar{\rho} \) configuration.

The evolutive equations for the energy components are obtained by using chain-rule differentiation and the equations of motion (Boussinesq). For example, the equation for \( \mathcal{E}_A \) is obtained as

\[
\frac{d\mathcal{E}_A}{dt} = \frac{\partial \mathcal{E}_A}{\partial \rho} \frac{d\rho}{dt} + \frac{\partial \mathcal{E}_A}{\partial R} \frac{dR}{dt} \quad (4.11)
\]

\[
= g \left[ y^*(R + \rho') - y^*(R) \right] u_i(R + \rho')/i \quad (4.12)
\]

\[
= g\eta u_i(R + \rho')/i + g \left[ y^*(R + \rho') - y \right] u_i(R + \rho')/i \quad (4.13)
\]

where \( \eta = y - y^*(R) \).

In what follows we shall mainly consider volume integrals over the fluid region \( \Omega \), denoted by \( \langle \cdot \rangle \), with the natural definition

\[
\langle f \rangle(t) \equiv \int_{\Omega} f(x,t) dV.
\]
By applying the \langle \cdot \rangle operator to equation (4.13), and performing the following manipulation

\[ g\langle y^*(\rho)u_i\rho/i_i \rangle = g\langle G_\rho(\rho)\rho/i_i u_i \rangle = g\langle G/u_i \rangle = 0, \]

where \( G_\rho = y^*(\rho) \), we obtain

\[ \langle \delta_\Lambda \rangle_t = g\langle \eta u_i'(R + \rho'),i_i \rangle + g\langle u'_2\rho' \rangle + g\langle u'_2R \rangle. \]

Notice that in both (4.15) and the above formula we used the divergence theorem, observing how the resulting boundary terms vanish under the present boundary conditions.

We can bring (4.16) into a form which is symmetric to the corresponding equation for the kinetic energy part (i.e. get rid of the terms containing \( R \)) by going through the following steps

\[ -\int \Omega \eta_{i/i}u_iRdx dy + \int \Omega u_2Rdx dy = \int \Omega (y - \eta)_{i/i} u_iRdx dy \]
\[ = \int \Omega Ru_i\hat{n}_i ds d\phi = 0. \]

After a trivial first step, in the second one we have performed a change of variables \((x, y) \rightarrow (s, \phi)\), where \( s \) is an arclength coordinate along the base-flow streamlines and \( \phi = y - \eta = \psi/c_W \) is the scaled streamfunction (that dimensionally would have the units of a length).

By considering the local orthogonality between coordinate lines of \( s \) and \( \phi \), at any point there is an orientation with respect to which the Jacobian of the coordinate transformation is diagonal with entries 1 and \(|\nabla \phi|\). It follows the infinitesimal volume
transformation
\[ dx dy = \frac{ds d\phi}{\det(J)} = \frac{ds d\phi}{|\nabla \phi|} = \frac{ds d\phi}{|\nabla \eta - y|}, \]
used to obtain the second equality. The last equality follows from choosing to integrate in \( s \) first (Fubini’s theorem) and then observing how the diapycnal volumetric flux must vanish \( \int R(\phi)u_i \hat{n}_i ds = R \int u_i \hat{n}_i ds = 0 \). The above derivation and others similar for the rest of the energy components, lead to the set of energy budget equations:

\[ \langle E_K \rangle_t = -\langle u'_i u'_j U_{i,j} \rangle - g \langle u'_2 \rho' \rangle, \]  
\[ \langle E_A \rangle_t = g \langle u'_2 \rho' \rangle \]  
\[ \langle e_K \rangle_t = \langle u'_i u'_j U_{i,j} \rangle - g \{ \langle \rho' U_2 \rangle + \langle u'_2 R \rangle \}, \]  
\[ \langle e_A \rangle_t = -g \langle u'_i \rho' \rangle + g \{ \langle \rho' U_2 \rangle + \langle u'_2 R \rangle \}, \]

where physically \( \langle e_K \rangle \) and \( \langle e_A \rangle \) represent the (non positive-definite) variation of the energy stored in the background state. All the energy exchange paths are sketched in figure 4.2. The structure is the same as the one reported by [65].

We further notice that for parallel flows the balance takes the simpler form

\[ \langle E_K \rangle_t = -\langle u'_i u'_j U_{i,j} \rangle - g \langle u'_2 \rho' \rangle, \]  
\[ \langle E_A \rangle_t = g \langle u'_2 \rho' \rangle \]  
\[ \langle e_K \rangle_t = \langle u'_i u'_j U_{i,j} \rangle, \]  
\[ \langle e_A \rangle_t = 0 \]

with \( \langle e_A \rangle_t = 0 \) identically. This reflects the fact that in parallel shears the background density stratification is the minimal potential energy configuration itself (\( \eta = 0 \)), so that no available potential energy can be extracted by the perturbations. In this case
Figure 4.2: Schematic of the energy transfer across the four constituent parts of the total energy. Our convention for the sign of the transfer terms is indicated by the arrows. The solid-line connections mark the transfers allowed in parallel shears.

$\langle E_A \rangle$ can only exchange energy with $\langle E_K \rangle$, resulting in a reduction of the allowed energy transfers.

**Explicit expression for $E_A$ in the tanh-stratification case.** When the undisturbed stratification is set to vary between an upper and a lower value ($\rho_1$ and $\rho_2$ respectively) as

$$\bar{\rho} = \frac{\rho_2 + \rho_1}{2} + \frac{\rho_1 - \rho_2}{2} \tanh[(y - y_0)/\delta]$$

the expression for $E_A$ can be made explicit. By inverting the hyperbolic tangent we first obtain

$$y^*(\rho) = y_0 - \frac{1}{2} \delta \log \left( \frac{\rho - \rho_1}{-\rho + \rho_2} \right).$$

The integral in (4.9) can then be easily computed to obtain

$$E_A = g I(R + \rho', y^*(R + \rho')) - g I(R + \rho', y^*(R)),$$

where

$$I(\rho, y) = -\rho y + \frac{1}{2}(\rho_1 + \rho_2)y + \frac{1}{2} \delta(\rho_1 - \rho_2) \log \left[ \cosh \left( \frac{y - y_0}{\delta} \right) \right].$$

The construction of $\mathcal{R}$ also follows easily.
Figure 4.3: Horizontal velocity perturbation (left) and density perturbation (right) from parallel shear simulation. The lines reference the same levels of background density as in figure 4.1 ($R = 1.05, 1.015$), the labels inside left panels indicate time.
Figure 4.4: (a) Time evolution of integrated energy components computed from numerical simulations for the parallel-shear background. The curves are: $\langle E_K \rangle$ solid-blue, $\langle E_A \rangle$ dashed-red, $\langle e_K \rangle$ solid-grey, $\langle e_A \rangle$ dashed-grey, total sum solid-black-thick. (b) Volume-integrated energy budget terms versus time. The curves are: $P_K$ solid-black, $P_A$ dashed-black, $C_{KtoA}^E$ solid-grey, $C_{KtoA}^e$ dashed-grey, and $P_K - C_{KtoA}^E$ dash-dot. Markers are the time-derivatives of $\langle E_K \rangle$ and $\langle E_A \rangle$ computed through interpolation. Notice that $\langle e_A \rangle$, $P_A$, and $C_{KtoA}^e$ are identically null in this case (line-styles are given for future reference).

4.2.2 The parallel shear case

We use the tanh-shear model for the parallel flow simulations, with parameters chosen to realize marginally stable conditions, see table 4.1. This is convenient for comparisons, in §4.2.3 and §4.2.4 below, with the more complicated case of perturbations evolving within the spatially increasing case of self-induced shear upstream from the wave maximum. In the scaling used in §2.1 we have $V = 0.1$, $\sigma = 0.01$, $\ell = 0.05$, $g = 9.8$, and $J = 0.49$, which is close to the conditions met by the W1 around the inflection point of the wave’s profile. The streamwise wavenumber $k = 10$ ($k = 1/2$ in the scaling of §2.1), corresponds to the point in the stable region closest to the stability boundary.

The initial condition for this simulation consists of the above shear flow with a superimposed perturbation. To mimic our main case of interest, as described in §4.1.1, the perturbation is again the first baroclinic mode of the stratification. Thus, the
evolution can be thought of as the effect of a shear flow being suddenly switched on, thereby rearranging the initial modal structure. The resulting flow is visualized in figure 4.3, and these snapshots readily suggest that the evolution can be organized in two different phases.

During the first phase \( t \lesssim 3 \) the flow structure undergoes a radical reorganization, with the initial structure being depleted until the disturbance settles on a stack of nearly-horizontal filaments. Thereafter a second phase sets in, with the flow maintaining the same type of structures, which however are made increasingly thinner by the shear action. Observing the late frames in figure 4.3 \( t = 10.2 \) and \( t = 16.4 \) shows that the filaments are clustered underneath the mean density isoline of the background stratification. Such peculiar downward-pointing arrangement bears some memory of the initial condition, which is chosen to be the right-traveling mode (indeed it would be opposite – upward-pointing – if the perturbation were chosen to be the left-traveling mode).

Figure 4.4 shows the time history of the perturbation energy and budget. Since the perturbation is initialized as an eigenmode of the shear-free background, the energy starts off equally distributed between the kinetic and the potential part (Yih 1960). At the earlier times of the evolution a growth of the perturbation energy takes place, especially evident in \( \langle E_A \rangle \). This stage corresponds to the depletion of the initial spatial structure of the baroclinic mode, see visualizations in figure 4.3. In the subsequent phase, the evolution of the perturbation energy settles on a monotonic decay. This corresponds to the stage in which the flow structures are organized in thin stretching filaments. It is interesting here to note a close analogy with an exact solution available in the case of uniform shear on linear stratification, and discussed by [38] as a case of transient non-normality effects. Such solution, similarly to the present one, consists of stretched bands and yields long-time energy decay after an early-time transient growth.
Figure 4.5: Blow-up of the region near the maximum slope of the pycnocline for the snapshots in figure 4.1, showing (a) horizontal velocity and (b) density perturbations. Notice the different times (labeled in panel (a)) with respect to figure 4.1 to better zoom in on the entrainment phase.

Figure 4.6: Same as figure 4.4, but for run W1R.
The sum of all energy components, which is conserved by the inviscid equations of motion, is a convenient tool to assess the quality of the numerical computation. The conservation of total energy is satisfactory, with only a slight variation well within the range (1%) of the error introduced by the Boussinesq approximation in our energy balance. A further check on convergence is offered by figure 4.6b, where the time derivatives of the energies computed by time-interpolation of the simulation data are compared with the corresponding fluxes directly computed from their expressions in (4.25). As one can see, the agreement among these quantities is again quite satisfactory.

In the next section we contrast the above parallel shear evolution with the entrainment phase in the wave-induced shear layer. The intensification of the background shear underlying a downstream-advected perturbation then results in effects mirroring those described above. This provides evidence that the non-orthogonality of the eigenmodes is playing a significant role in the entrainment dynamics.

4.2.3 Self-induced shear by internal waves: the locally stable case

We now introduce (non-parallel) space dependence into a shear flow making sure to avoid the additional complications resulting from the presence of an unstable eigenvalue branch within the flow. Thus, by choosing the background flow from an internal wave with no unstable shear pocket, we isolate non-normal and non-parallel mechanisms from the local unstable growth. (Of course, the neutral stability of the spectrum does not imply absence of evolution.) The background wave W1 in table 4.1 is expected to meet such requirements as \( \text{Ri} > 1/4 \) everywhere provides a good indication of stability, and in fact no local instability was detected by the model (figure 3.3a). Run W1R, which we used as a motivation in §4.1.1, will now be examined in greater detail, see figure 4.5. The density isolines help in recognizing the similarities between the structures that develop in this case and the structures observed in the parallel case, again correlated to the
direction of propagation of the baroclinic mode chosen for the upstream perturbation.

The energy evolution for this nonparallel case is reported in figure 4.6a, with the corresponding energy budget terms depicted in 4.6b. The scale of perturbation energies can be compared with those of the background internal wave by referring to table 1. The perturbation energies $\langle \mathcal{E}_K \rangle$ and $\langle \mathcal{E}_A \rangle$ decrease monotonically in time. Such decrease occurs during the entrainment phase of the perturbation within the wave-induced shear (roughly, for time $15 < t < 25$), while the perturbation interacts with the increasing shear of the flow (cf. figure 4.5.) The most evident differences between the parallel and the (wave-induced) non-parallel shear lie in the startup dynamic, with stronger coupling to the background flow for the non-parallel case during this phase. The evolution of $\langle e_K \rangle$ and $\langle e_A \rangle$ is more involved, as more means of energy transfers are allowed in the non-parallel case, as mentioned in §4.2.1. In particular, $\langle e_A \rangle$ is no longer forced to be constant. Note that even in the non-parallel case conservation of the total energy is maintained up to a substantial level of accuracy. Over the fairly long time scale of the simulation, the total-energy drops by $\approx 4\%$. This gives an indication of how the numerical simulation of thin-pycnocline waves is indeed particularly demanding in terms of numerical resolution. Figure 4.6b shows that in the non-parallel case variations of $\langle \mathcal{E}_A \rangle$ are driven by three terms. The overall result is a decrease of this quantity, with $\langle \mathcal{E}_A \rangle$ mediating an energy transfer between $\langle e_K \rangle$ and $\langle e_A \rangle$. Note that even after $\langle \mathcal{E}_A \rangle$ settles on a constant value it still mediates transfer from $\langle e_A \rangle$ to $\langle e_K \rangle$.

An appealing interpretation of the scenario just described is suggested by the spectral analysis in §3.1 (figure 3.3a), where we have shown the clustering of the neutral spectrum on the velocity extrema as the shear develops. The clustering suggests an effective spreading of energy among neutral modes, which in turn can give rise to non-normal effects.
4.2.4 Self-induced shear by internal waves: the locally unstable case

By making the pycnocline thinner (wave W2 in table 4.1) an instability pocket, i.e., a region where the $R_i < 1/4$, develops within the wave-induced shear. According to the $R_i$ criterion, in this case it becomes possible to observe the third mechanism of local unstable growth within the classification given in the opening of this chapter. Indeed, the interval of $x$-values where the model detects an unstable eigenvalue (figure 3.3c) closely matches the instability pocket shown in figure 4.7. This figure also shows a bias of the $R_i < 1/4$ region to extend further towards the upper part of the pycnocline, a consequence of the milder density gradient for the upper layer which is also captured by the asymptotic model (3.9) and (3.8), see figure 3.4.

By replicating the same numerical experiment from the previous section on W2 (run W2R1), we find that the disturbance does not experience any growth during the crossing of the instability pocket: the perturbation is effectively damped in the same fashion as it was in both the parallel shear and the stable wave-induced shear. This seems at odds with the presence of the unstable shear-flow pocket for this case. We report in figure 4.9a the corresponding time evolution of the perturbation energy: its behaviour is almost identical to the case of the stable wave-induced shear displayed in figure 4.6a.

This result seemingly points to the conclusion that even with an instability pocket the shear behaves as it were stable. Previous studies (Barad & Fringer 2010, Fructus et al. 2009) support the fact that the instability pocket needs to extend widely for the shear
Figure 4.8: Same as figure 4.1 now for runs W2R1 (a) and W2L1 (b) in table 4.2. Notice that unstable growth takes place only in case (b).
Figure 4.9: Same as figure 4.4, now with non-parallel shear background flow from W2 wave. (a),(b) W2R1 (c),(d) W2L1. Note the different scales between the plots.
instability to be observable. However, our next result shows that the interplay between the spatial extent of the instability pocket and the nature of the perturbation may be more subtle, and can exhibit strong dependence on the perturbation itself: for the very same choice of parameters (and hence identical instability pockets), a different choice of the upstream perturbation leads to a very different outcome.

By simply selecting the left-traveling baroclinic (W2L1) mode as the packet carrier instead of the right-gong, we now observe strong growth in our energy diagnostics, see figure 4.9c and 4.9d for the budget. These figures show how the disturbance growth involves a transfer of energy from the background flow to the perturbation via both the kinetic and potential energy terms; as remarked in the previous W1-case, the second type of transfer is a non-parallel effect. Not unexpectedly, this is reflected in the snapshot from the simulation depicted in figure 4.8. The presence of the unstable Kelvin–Helmholtz mode’s growth past the wave maximum is quite noticeable, although the instability is still in its linear growth phase with no fully developed roll-ups. (The initial amplitude of the perturbation is small enough to prevent instability from saturating and form billows before the perturbation reaches the end of the instability pocket.)

As we observe unstable growth, we also verify its connection with the locally unstable character of the shear in the W2 wave. In fact, by choosing to perturb the W1 wave with the left-travelling mode (run W1L) no comparable effect is triggered, apart from a slight time delay, see figure 4.10.

These observations confirm the convective nature of the instability (as opposed to absolute instability, see, e.g., Huerre & Monkewitz 1985 for a definition) for internal waves, at least for the range of parameters we have studied. Thus, the semi-empirical instability criteria presented by various authors are likely to be affected by a specific level of noise. We remark that the analysis by [53] supports the fact that absolute instability can arise only for very different values of parameters, in particular for den-
sities of the lighter fluid that are low enough to reduce the setup to essentially a single free-surface fluid.

4.2.5 Interpretation in terms of spatial spectrum

The evidence that local unstable growth takes place only in run W2L1 implies that the local growth rate of temporal instability $\omega_I$, for a fixed $k = k_B$, fails to be a robust predictive criterion for the occurrence of unstable growth. Together with the observation of convective instability, this suggests that a spatial, as opposed to temporal, stability study might be more appropriate for the internal wave self-induced shear. The spatial approach also can be justified on a more theoretical basis using some basic elements of slow-varying flow asymptotic analysis. In the framework of slow-varying media the law of conservation of frequency

$$\omega_T + c_g \omega_X = 0, \quad (4.26)$$

where $c_g = d\omega/dk$ is the group velocity, holds at leading order for modulated packets. In the above formula, we use the stretched coordinates typical of slow-media analysis, i.e., $X = \epsilon x$ and $T = \epsilon t$, where $\epsilon \ll 1$ is the long-wave parameter of small vertical vs.
horizontal scales. Our choice of perturbation (4.4) implies

\[ \omega = \omega_0^\pm \equiv k_B[c_W \pm c_0(k_B)] \quad \text{at} \quad t = 0 \]

and, according to (4.26), frequency is preserved at all times. Upon such considerations we can expect the linear response to behave like a signalling problem at leading order approximation.

A computation of the spatial spectrum at the wave maximum (located at \( x = 8 \),
Figure 4.13: Direct comparison of perturbation growths for all runs using the W2 background, the quantity plotted is $\langle E_k \rangle$. Notice log scale.

i.e., solving (3.15) for $k$ keeping $\omega = \omega_0^\pm$ fixed (figure 4.12), indeed detects spatial instability only for case W2L1. We proceed to test spatial stability by designing two more runs. Unlike the perturbations used in W2L1 and W2R1, which were targeting wavenumbers in the middle of the temporal instability $k$-range for unstable shear pockets, we now choose initial values of $\omega_0^\pm$ that would lead to nonzero imaginary $k$ components according to the conservation law (4.26) and the model dispersion relation (3.15). Hence, we look at the baroclinic modes and seek different values of $k_B$ yielding the same frequency by the dispersion relation. This is illustrated in figure 4.11, which shows how runs W2L2 and W2R2 are defined. A direct comparison of all four W2-runs is shown in figure 4.13. Case W2R2, which shares the frequency $\omega_0^-$ with case W2L1, clearly manifests growth, even though this is milder than in the latter case. On the other hand case W2L2 exhibits only energy decay similar to that of the W2R1 case.

The quantitative difference noticed between the two cases showing perturbation growth can be ascribed to the non-normal entrainment dynamic preceding the growth of the instability, which ultimately results in different magnitude of the excitation source in the instability pocket (notice the energy decrease for $15 < t < 25$ that has no counterpart in W2L1 in figure 4.13). Figure 4.14a confirms how, in both runs W2L1 and
Figure 4.14: (a) Fourier power spectra of the 1-dimensional signal obtained by evaluating $\rho'$ along the isopycnal $R = (\rho_1 + \rho_2)/2$, taken at $t = 0$ and at the time corresponding to the maximum amplification for each run. (b) Similar plot for run W2R1. The isopycnal is displaced downward, $R = 1.017$, to better focus on the features of interest (cf. discussion).
W2R2, the observed growth is to be attributed to the spatial instability of the same $k$-mode. In fact, when the disturbance reaches its maximum ($t \approx 43$ for W2L1, and $t \approx 40$ for W2R2), the peak of the streamwise Fourier spectrum of the disturbance, in suitable one-dimensional representation, migrates toward the wavenumber corresponding to the spatial eigenvalue (observe that $k_R(\omega_0^-) \approx 12$ in figure 4.12). The plot also quantifies how the characteristic wavenumber of the wave packet visible in the last frame of figure 4.8b ($t = 36.4$) has varied from its initial value in the first frame.

In closing, it is important to remark that the pure spatial growth viewpoint is only an approximation, as the spatial growth of the instability cannot continue indefinitely due to the finite extent of the unstable shear pocket and time evolution must also occur. Spatial and temporal spectra can be linked in a simple way when perturbations carried by the neutral modes, hence those undergoing non-normal effects, are concerned. As figure 3.3b shows, the clustering of neutral-mode eigenvalues $c_n$ onto the end of the velocity range is a robust feature about the wave maximum. One can then postulate that any perturbation carried by neutral modes is eventually advected by either one of the shear limiting velocities $U_1$ or $U_2$, or $c = \omega/k \rightarrow U_{2,1}$, and obtain the very simple relation

$$k \approx \omega_0^+/U_{2,1}. \quad (4.27)$$

For example, with run W2R1, and so $\omega = \omega_0^+$, this criterion predicts that a typical $k$ value for the small perturbations visible below the pycnocline in the last two frames of figure 4.8a should be $k \approx \omega_0^+/U_2$ (or $k \approx 14$ by picking $U_2 = 0.3$). This assumes that the perturbation is carried primarily by the neutral modes limiting onto the initial baroclinic mode. Because of the velocity-interval gap $[U_1(x), U_2(x)]$ in the spectrum as the shear develops, these modes are the ones limiting from above onto the curve $U_2(x)$ in figure 3.3b. We remark that the same argument can be applied to predict the wavenumber $k_R$ detected in the spatially unstable cases W2L1 and W2R2, by considering the
mean velocity \((U_2 + U_1)/2\) in place of \(U_{2,1}\) in the approximate relation (4.27) above. The Fourier power spectra in figure 4.14 confirm how such a simple estimate produces reasonable predictions, and suggests an operative criterion for experimental data analysis.

4.3 Discussion of results

The aim in this chapter has been to pin down some important aspects of the response of large internal waves to upstream perturbations. Using numerical simulations it was shown how the onset of shear instability for such flows is a significantly more subtle mechanism than its parallel counterpart.

The following scenario emerges from the numerical results presented in this section and those developed in previous chapters. Upstream perturbations initially located in the quiescent state upstream of the wave-induced shear region, can be decomposed into the basis of (orthogonal) neutrally stable baroclinic modes corresponding to purely discrete spectrum of the linearized motion equations. In §3.1 we have shown how this neutral spectrum deforms smoothly as the shear induced by the presence of a solitary internal wave intensifies. In this process the corresponding eigenmodes lose orthogonality, as the stability operator loses self-adjointness. In the wave reference frame, the baroclinic spectrum can thus be viewed as organized in spatially dependent branches of eigenvalues and (non-orthogonal) eigenmodes. In §4.2.2 we have considered the evolution of perturbations in a parallel shear; by distributing the perturbation energy among non-orthogonal eigenmodes it was possible to isolate the effect of non-normality that can lead to perturbation decay. Subsequently, the numerical simulations in §4.3-4.4 show that the same process leads to a significant depletion of the perturbation energy also in the non-parallel wave-induced shear. This energy is absorbed into the background flow in a process that can be viewed as an entrainment of an upstream perturbation.
within the wave-induced shear region. The process of perturbation absorption by the background wave can be locally reversed if the shear possesses pockets of instability, which occurs around the wave maximum for sufficient wave amplitudes and sufficiently thin pycnoclines.

To allow closed form expressions for the spectrum of the wave-induced shear flow, and obtain its dependence along a solitary wave profile, we have presented in section §3.1 a simplified model for the basic flow that allows for fast and accurate computation of the above spectrum, bridging with a continuous density transition the two-layer model of [29]. The new model reproduces reasonably well the wave structure from the fluid’s equilibrium state parameters. In particular, it captures the skewness of the density transition in the pycnocline, which in the numerical TEW solutions always exhibits gentler gradients towards the upper fluid.

Analytical results are compared with direct numerical simulations of the evolution of a single-mode upstream perturbation. Around the inflection point of the wave profile, where the clustering of the neutrally stable eigenvalues increases dramatically (figure 3.3), a peculiar stretching and damping behavior is observed (figure 4.5), similar to that of a baroclinic single mode suddenly immersed in a parallel shear (figure 4.3). Also, it is worth remarking that such stretching mechanism may result in enhanced diffusion once viscosity and diffusivities of real fluids are properly accounted for (see Part II of this dissertation). This effect may be relevant even at the time scales of internal wave dynamics. Further study of this is left for future investigations.

The main features of perturbation entrainment persist for internal waves with locally-unstable regions where \( \text{Ri} < \frac{1}{4} \). As mentioned above, this class of waves can act as an amplifier of disturbances. However, we find that the amplification responds selectively to the nature of upstream perturbations. Remarkably, choosing a perturbation corresponding to right-propagating baroclinic modes leads to a net damp-
ing similar to the one observed for *stable* self-induced shears, while the left-traveling choice leads to detectable unstable mode growth inside the instability pocket (visualized in figure 4.8 and quantified by the energy plots in figure 4.9). This selectivity to unstable growth can be given an explanation by focussing on the spatial (as opposed to temporal) formulation for the local spectral stability. Within this framework, the unstable growth in figure 4.8b is interpreted as spatial growth associated with the presence of an imaginary component of the wave number $k$. This viewpoint is supported by the results reported in figure 4.13, which illustrates how unstable growth is set by the choice of frequency $\omega = \omega_0^\pm$ of the initial perturbation in the wave frame. This is because in this reference frame the background flow is time-independent and slowly varying in space, so that $\omega$ is conserved at leading order in slowly varying asymptotics, while $k$ may develop an imaginary component along the wave profile.

Finally, we stress how the set of runs presented in figure 4.13 cautions against using, without further refinements, a simple-minded criterion of unstable growth based solely on the time of residence of the disturbance in the instability pocket. This criterion assumes that, for the same growth rate $\omega_I$, longer residence times lead to larger amplification factors under unstable shear flows, making the manifestation of instability more prominent with respect to that of shorter residence times. Thus, in traveling through the whole span of the instability pocket, the right-going perturbation of run W2R2 may be expected to take a shorter time than the W2L2 left-going perturbation, yet it is only in the W2R2 case that any growth can be detected.
CONTINUOUS SPECTRUM AND NON-NORMAL TRANSIENT DYNAMICS

The numerical simulations presented in chapter 4 have shown how small perturbations propagating through wave-induced shear layers evolve in a non-intuitive way. As soon as the disturbance is affected by the presence of shear, its features appear qualitatively different from a single-mode evolution. The filamentation of perturbations (see figures 4.3 and 4.5), and the absorption of perturbation energy in the background flow represent evidence that energy spreads across several eigenmodes even if the disturbance is initialized on a single mode. In other words, the evolution becomes strongly multimodal. The local spectrum along internal solitary waves, discussed in chapter 3, also warns about this possibility: as shown in §3.2 (in particular from figure 3.3), the neutral modes tend to lock in frequency as the shear intensifies, suggesting the occurrence of some resonant interaction. All these ideas have been largely assessed in the previous chapter, however, a further and probably relevant element was not considered until now: the continuous spectrum (introduced in §2.1.2).

The possible excitation of modes belonging to the continuous spectrum adds one more element to the already complex theoretical scenario ensuing from wave-induced shears. In order to move a step in this direction, here we perform an analysis of the continuous spectrum of the Taylor–Goldstein equation and those solutions obtained by superposition of the corresponding generalized eigenfunctions in parallel shears. Al-
though limited to this specific setting, the following results confirm that the continuous spectrum is deeply connected to the “damping-by-filamentation” mechanism observed.

The analysis presented in this chapter can be regarded as an extension of some previous results, in particular those of Farrell & Ioannou [38]. These authors have established that stratified shear layers can damp or enhance small perturbations even if the shear is linearly stable. In the field of flow stability it is well established [83] that whenever the underlying spectral operator is not self-adjoint, the non normality of eigenfunctions provides a mechanism for perturbation growth or decay, which is independent from spectral (in)stability itself. This avenue of research has recently received growing interest in many areas (e.g., stability of boundary layers and wall-bounded shear flows), but little is known as yet for stratified flows.

5.1 Singularities of the continuous spectrum eigenfunctions

The generalized eigenmodes of the continuous spectrum have been introduced in §2.1.2, some of their properties are now discussed in deeper detail.

The Frobenius expansion in $c$ of the continuous spectrum modes has the same structure as the $y$-expansion (2.5), i.e., it is obtained by replacing $y - y_c(c)$ with $c - U(y)$, and using the same indicial exponent, now regarded as dependent on $y$ as a parameter, $
u = \nu(y) = \left(\frac{1}{4} - \text{Ri}(y)\right)^{1/2}$. This can be directly verified by using such expansion inside (2.3) and obtaining an analogous recursive relation. As an alternative, one can fix $\omega = ck$ and regard $k$ as a free parameter. Also in this case, with $\phi = \phi(y, k)$, Frobenius expansions in either $(y - y_c(k))$ or $(k - k_c(y))$ hold, with $\nu = \nu(k)$ or $\nu = \nu(y)$ respectively. Note that the critical points, $y_c$ and $k_c$, correspond to a regular singularity in the differential equation (2.3), provided $U_y(y_c) \neq 0$. If this is not the case, the local behavior of the solution degenerates into an essential singularity, which greatly increase the analytical challenge. We shall not consider this possibility assuming $U_y(y) \neq 0$ everywhere (a condition met in many cases of concrete interest, including wave-induced
shear flows).

We choose to normalize eigenfunctions on the coefficient of the leading exponent in the $y$-expansion, i.e., by setting

$$|a_0| = 1 \quad \text{and} \quad b_0 = \overline{a_0}. \quad (5.1)$$

In the calculations presented next it will be necessary to know what the coefficients of the leading-order terms in both the $c$- and $k$-expansions are under this normalization. The conversions between the coefficients of the different expansions are obtained from the leading term in the Taylor expansions of $(c - U(y))$ and $(k - k_c(y))$ around $y_c$

$$c - U(y) = c - \left[ U(y_c(c)) + U_y(y_c(c))(y - y_c) + \mathcal{O}((y - y_c)^2) \right] \quad (5.2)$$

$$= -U_y(y - y_c) + \mathcal{O}((y - y_c)^2) \quad (5.3)$$

$$k - k_c(y) = k - \left[ k_c(y_c(k)) + \frac{dk_c}{dy}(y_c(k))(y - y_c) + \mathcal{O}((y - y_c)^2) \right] \quad (5.4)$$

$$= \omega U_y U^2 (y - y_c) + \mathcal{O}((y - y_c)^2) \quad (5.5)$$

then

$$\hat{\phi}_k^\pm(y, c) \sim a_0 \left( -\frac{c - U}{U_y} \right)^{1/2 + \nu} + b_0 \left( -\frac{c - U}{U_y} \right)^{1/2 - \nu}, \quad \text{for} \quad c \rightarrow U^\pm \quad (5.6)$$

and

$$\hat{\phi}_k^\pm(y, k) \sim a_0 \left( \frac{U^2}{\omega U_y} (k - k_c) \right)^{1/2 + \nu} + b_0 \left( \frac{U^2}{\omega U_y} (k - k_c) \right)^{1/2 - \nu}, \quad \text{for} \quad k \rightarrow k_c^\pm(y). \quad (5.7)$$

A comparison between “exact” generalized eigenfunctions and their local Frobenius expansions is reported in figure 5.1. The eigenfunction are computed numerically (see §5.3.1 for details), notice how these plots confirm the accuracy of the numerical
computation in a neighborhood of the singular points.

Figure 5.1: Examples of continuous spectrum modes (blue symbols) compared to the leading order Frobenius expansions (purple symbols) given by (5.6) and (5.7). Eigenfunctions $\hat{\phi}_k^+(y, c)$ (top) and $\hat{\phi}_\omega^+(y, k)$ (bottom) as a function of $c$ and $k$ respectively, for $y = 0$.

5.2 Continuous-spectrum solutions

We consider solutions of the linearized equations on a parallel shear obtained by superposition of the generalized eigenfunctions only. The general continuous-spectrum
solution is given by

$$
\hat{\Phi}(x, y, t) = \int_{-\infty}^{+\infty} \int_{U_{\min}}^{U_{\max}} H^\pm(k, c) \phi^\pm(y, k, c) e^{ik(x-ct)} dc dk,
$$

where $H^\pm(k, c)$ represents the coefficients of the linear superposition, determined by specific initial conditions, and the superscript $\pm$ references either left- ($-$) or right-handed ($+$) eigenfunctions. Notice that the generalized eigenfunctions are individually weak solutions of the Taylor–Goldstein equation; however, if $H$ is a suitably smooth function, $\hat{\Phi}$ is a smooth (hence strong) solutions of the linearized equations of motion.

The above construction gives rise to a broad class of solutions. Amid such a generality, we restrict our attention to individual “wave packets”, i.e., distributions $H^\pm(k, c) = \tilde{H}^\pm(s) = \delta(k-k'(s), c-c'(s))$ localized on an arbitrary path $\gamma$ parametrized by the arclength coordinate $s$ in the $(k, c)$ plane. In doing so, we obtain one-dimensional superpositions

$$
\hat{\Phi}_\gamma(x, y, t) = \int_\gamma \tilde{H}^\pm(s) \phi^\pm(y, k'(s), c'(s)) e^{ik'(s)(x-c'(s)t)} ds.
$$

The freedom in the choice of $\gamma$ allows to construct wave packets possessing arbitrary
dispersion relations $\omega = \omega(k)$. The canonical structure for dispersive wave packets can be obtained by transforming the above integral as

$$\hat{\Phi}_\gamma(x, y, t) = \int_{k_{\text{min}}}^{k_{\text{max}}} w_{\gamma}^\pm(k) \phi^\pm(y, k, c) e^{i(kx - \omega(k)t)} dk,$$

with $w_{\gamma}(k) = H(k, c(k))(d\gamma/dk)$, where $d\gamma/dk$ denotes the appropriate factor introduced by the change of integration variable. Tools of asymptotic analysis apply to the above integral for large values of $x$ and $t$. For instance, Whitham’s saddle-point analysis (or steepest-descent analysis [13]) allows to study the asymptotic behavior along rays $x/t = \text{const.}$ for long times. However, the singular kernel introduces considerable complications, due to competing contributions from both saddle points and singularities. For such reason we focus, from now on, on the two important limiting cases given by either $k = \text{const.}$ or $\omega = \text{const.}$. The corresponding paths $\gamma$ are shown in figure 5.2.

5.2.1 Temporal solutions

Solution of the first kind, $k = \text{const.}$, to which we shall refer as temporal solutions, can be written as

$$\Phi(x, y, t) = \hat{\Phi}(y, t)e^{ikx} + \text{c.c.},$$

with

$$\hat{\Phi}(y, t) = \int_{\text{min}(U)}^{\text{max}(U)} \hat{\phi}^\pm(y, c) w^\pm_k(c) e^{-ikct} dc. \quad (5.8)$$

The function $w_k(c)$ represents the coefficients of the linear superposition. The corresponding density field is given by

$$\hat{R}_k(y, t) = \int_{\text{min}(U)}^{\text{max}(U)} \hat{\rho}^\pm_k(y, c) w^\pm_k(c) e^{-ikct} dc \quad \text{with} \quad \hat{\rho}_k = \frac{\rho_0 N^2}{g} \frac{\hat{\psi}_k}{U - c}. \quad (5.9)$$
As one can see the eigenfunctions have a stronger singularity in the density field. Even though such singularity is integrable care must be taken when the above integral is discretized for computations, as will be discussed later. The features of the continuous-spectrum solutions are certainly not apparent from their definitions above, however such integral representations are amenable of much more informative asymptotic analysis, as we now show.

To start with, notice that for long times, $kt \gg 1$, the exponential inside the above integral becomes highly oscillatory. Under the sole assumption that $w^\pm(c; k)$ is an integrable function of $c$ inside $[U_{\text{min}}, U_{\text{max}}]$, it follows that

$$
\lim_{t \to \infty} \hat{\Phi}_k(y, t) = 0 \quad \text{and} \quad \lim_{t \to \infty} \hat{R}_k(y, t) = 0
$$

for any $y$ (Riemann–Lebesgue lemma). We shall further assume that $w^\pm(c; k)$ is analytic in $c$ and that $w^\pm \to 0$ as $c \to \max(U), \min(U)$. In this case the dominant contribution to the integral localizes around $c = U(y_c)$, the branch-point singularity of $\hat{\phi}$, so that the asymptotic decay rate is dictated by the leading term in the Frobenius expansion (2.5).

For general shear flows the long-time asymptotic expansion of (5.8) can be obtained by applying Watson’s lemma (Bender & Orszag 1999), which establishes that the long-time behaviour of an integral $I(t) = \int_0^b f(x)e^{-xt}dx$ is given by $I \sim \Sigma a_0 \Gamma(\alpha + \beta n + 1)x^{-\alpha - \beta n - 1}$ if $f$ possesses the asymptotic expansion $f \sim \Sigma a_0 x^{\alpha + \beta n}$ about $x = 0$. In order to apply this result, we must first deform the path of integration away from the real axis into the complex plane, as illustrated in figure 5.3. The contributions from the segments $C_2$ and $C_1$ are asymptotically subdominant, because on $C_2$ the integrand is uniformly exponentially small, $O(e^{-k|C_1|t})$ (where $|C_1| > 0$ is the length of $C_1$), while on $C_1$ the leading contribution comes from the upper extremum ($c = U_{\text{max}}$) where the integrand has (at most) a simple zero. Along $C_3$, after the change of variable
\(-i\ell = (c - U(y))\), the integral (5.8) becomes

\[
\hat{\Phi}_k(y, t) = \int_0^{-i|C_3|} \hat{\phi}_k^\pm(y, \ell) w_k^\pm(\ell) e^{-k\ell t} d(i\ell) \tag{5.10}
\]

\[
\sim i \left( \frac{i}{U_y} \right)^{1/2+\nu} \int_0^{-i|C_3|} \left( a_0 \ell^{1/2+\nu} + b_0 \ell^{1/2-\nu} \right) w_k^\pm(\ell) e^{-k\ell t} d\ell \tag{5.11}
\]

which is a canonical Watson integral. Direct application of Watson’s lemma then yields the following long-time solution

\[
\hat{\Phi}_k = W_a e^{-ikUt} |t|^{-\frac{3}{2} + \nu} + W_b e^{-ikUt} |t|^{-\frac{3}{2} - \nu} + \mathcal{O} \left( |t|^{-\frac{5}{2} + \nu} \right), \quad \text{as} \quad |t| \to \infty, \tag{5.12}
\]

with

\[
W_a(y) = i \left( \frac{i}{U_y} \right)^{1/2+\nu} w^\pm(U(y)) \Gamma \left( \frac{3}{2} + \nu \right),
\]

and

\[
W_b(y) = i \left( \frac{i}{U_y} \right)^{1/2-\nu} w^\pm(U(y)) \Gamma \left( \frac{3}{2} + \nu \right).
\]

Such asymptotic solution consists in bands being stretched and absorbed by the shear similarly to the exact solution for linear shear and stratification. The stretching rate however is not uniform across the flow, but depends on the local conditions of the base flow. It should also be noticed that for \( t < 0 \) the dynamic takes place in reverse: the
filaments are compressed as they are inclined in the sense opposite to the shear strain, and this process leads to growth of the perturbation instead of decay.

We remark how in the specific case of homogeneous stratified shear, $U(y) = y$ and $N^2 = \text{const.}$, the present analysis recovers the results from an analysis by Farrel & Joannoui (1993). Under these assumptions the eigenfunctions are translation-invariant, i.e., $\hat{\phi}_k^\pm(y, c) = \hat{\phi}_k^\pm(\xi)$ with $\xi = y - c$. By setting $w^\pm(c, k) = -ilc$ the integral (5.8) becomes

$$\hat{\Phi}_k(y, t) = e^{i(y(l - kt))} \int_{-\infty}^{\infty} \hat{\phi}_k^\pm(\xi; k) e^{i\xi(l - kt)} d\xi,$$

which recovers the ansatz that in Farrel & Joannoui (1993) is assumed and then used directly in the linearized Boussinesq equations to obtain an evolution equation for $\Upsilon(t)$ ($\hat{\psi}$ in their notation). Long-time analysis of such differential equation leads to the asymptotic algebraic decay rate $\Upsilon(t) \sim t^{-3/2 \pm \nu}$ for $t \to \infty$. The assumption of linear background flow is essential in such calculation, hence the present analysis extends the same type of result to arbitrary shear and stratification profiles. Furthermore, it allows to construct a class of solutions which is the spatial analog of the solutions so far discussed, i.e., time-periodic perturbations with spatial decay, as shown next.

### 5.2.2 Spatial solutions

By considering paths $\gamma$ on which $\omega$ is constant we obtain spatial continuous-spectrum solutions. Such solutions, which contain all wavenumbers $k$ given by $k = \omega/c$ for $\omega$ fixed and $c$ in the range of $U(y)$, are time-periodic

$$\Phi(x, y, t) = \hat{\Phi}_\omega(x, y)e^{-i\omega t} + c.c.$$
In order to avoid the singular case in which $k$ can diverge to infinity, we assume that $U(y) > 0$ everywhere. Such assumption, which simply sets the system of reference, implies that such class of solutions consists of traveling wave packets if the flow velocity changes sign. The wavenumber then varies in the range $k \in [\omega/U_{\text{max}}, \omega/U_{\text{min}}]$, and we can construct solutions as

$$
\hat{\Phi}_\omega(x, y; \omega) = \int_{\omega/U_{\text{max}}}^{\omega/U_{\text{min}}} \hat{\phi}_\omega^+(y, k) w_\omega^+(k) e^{ikx} dk.
$$

(5.13)

The procedure developed in the previous section, yielding the long-time behavior of the $\hat{\Phi}_k$ solutions, applies verbatim to the present case after swapping the roles of $x$ and $t$. The same type of calculation now yields the following result

$$
\hat{\Phi}_\omega = W_a|x|^{-3/2+\nu(y)} + W_b|x|^{-3/2-\nu(y)} + \mathcal{O}(x^{-5/2+\nu(y)}) \quad \text{as} \quad |x| \to \infty,
$$

(5.14)

with

$$
W_a(y) = \left( \frac{iU^2}{\omega U_y} \right)^{1+\nu} w^+ \Gamma \left( \frac{3}{2} + \nu \right),
$$

and

$$
W_b(y) = \left( \frac{iU^2}{\omega U_y} \right)^{1-\nu} w^\pm \Gamma \left( \frac{3}{2} + \nu \right),
$$

which is the analog of (5.12) for long distance in space (recall the assumption $U_y \neq 0$).

Figure 5.6 contains an example of a $\hat{\Phi}_\omega$ solution, obtained numerically by discretizing the values of $c$ on a grid, computing the eigenmodes with an ODE solver for any $c$, and then approximating the integral (5.13) with a discrete summation. As the picture shows, the same mechanism of growth/decrease associated with compression/stretching of the perturbations found in the temporal case is present also in this case, with evolution taking place in space.
Figure 5.4: Time frames of a $\Phi_k$ solution with $w^+ = e^{-8(y_c(c))^2}$, $w^- = 0$ and $k = 2/3$.

Figure 5.5: A $\Phi_\omega$ solution with $w^+ = e^{-8(y_c(\omega/k)+1/2)^2}$, $w^- = 0$ and $\omega = 2$. Top panel shows streamfunction, bottom panel density. For the background shear parameters see the caption of figure 2.3.

5.3 Numerical verification

In order to demonstrate the validity of the above analysis direct numerical tests are performed. The continuous-spectrum solutions are constructed numerically and implemented as initial conditions for the direct Euler solver VARDEN. For obvious computational reasons, the domain extension must be finite, and a cut-off must be applied to the functions $\Phi_\omega$ and $\hat{R}_\omega$ in the $x$ direction. We expect to observe a numerical solution that behaves as the time-periodic ideal solution over a sufficiently long time scale, before boundary effects as well as other numerical errors will eventually cause deviations from the ideal case. We present one example, based on the case of spatial solutions.

Figure 5.7 shows the result from a simulation in which the spatial continuous-spectrum solutions are superimposed as small perturbations on the corresponding par-
Figure 5.6: Comparison between “exact solutions” constructed numerically (markers) and the asymptotic expansions (lines). Left panel: time evolution of the temporal solution reported in figure 5.4 taken at $x = 0$ and $y = -0.33$. Right panel: horizontal slice of the spatial solution reported in figure 5.6 taken at $y = -0.57$ and $t = 0$.

allel shear background, which in this case is defined by

$$U(y) = 2 + \tanh(y), \quad R(y) = \frac{\rho_2 + \rho_1}{2} + \frac{\rho_1 - \rho_2}{2} \tanh(y)$$

with $\rho_1 = 0.966$ and $\rho_2 = 1.034$ and $g = 9.8$. The corresponding overall Richardson number is $J = 0.35$ (stable conditions). In this case $\Phi_\omega$ and $\tilde{R}_\omega$ have been smoothly sent to zero after $|x| > 30$. This ensures a wide observation window inside which the solution appears periodic over several time periods $2\pi/\omega$. The computational domain size is $L_x \times L_y = 64 \times 4$, with a grid spacing $h = 1/32$. The number of eigenfunctions employed to construct the initial condition is $N_c = 385$, see the next section for a discussion of this procedure. The plot reported in figure 5.7 is an excellent confirmation of the theory, as the simulation behaves effectively as the ideal periodic solution over the time scale shown.

5.3.1 Computational issues

The continuous spectrum solutions are constructed numerically by using quadrature rules on the integrals (5.8), (5.9) and (5.13). As already mentioned, an accurate
Figure 5.7: Demonstration of time-periodic behavior for a spatial solution in a full numerical simulation using VARDEN. It is shown the time evolution of an horizontal slice of the density field taken at $y = 0$. The portion shown corresponds to $-14 < x < 14$ and $0 < t < 18.8$, which spans about 6 periods with $\omega = 2$.

evaluation of such integrals requires some care, as the integrands contain singularities. In what follows the entire procedure is summarized, referring to the temporal solution, i.e. (5.8) and (5.9), as an example. (The same procedure applies to the spatial case without any substantial change.)

First, it is introduced a set of discrete values $c_n = U(\hat{y}_n)$, with $n = 1, 2, ..., N_c$, and $\hat{y}_n$ corresponding to an even grid of $y$ values. For any $c_n$ the eigenfunctions where computed solving the Taylor–Goldstein equation with an ODE solver package. The numerical integration is started from a boundary (upper for $\hat{\phi}^+$, lower for $\hat{\phi}^-$) and terminated close to the singular point $y_c(c_n)$. Attention must be paid in order to ensure a solution accurate in a small neighborhood of $y_c$, however, since nowadays all the popular software packages provide very accurate adaptive ODE solvers this can be accomplished with very limited efforts. Eigenfunction are normalized according to (5.1), and reported on a grid of $y = y_n$ values, $n = 1, 2, ... N_y$, obtaining a discretization of the
functions $\hat{\phi}^+(y, c)$ on a rectangular grid $[1, ..., N_y] \times [1, ..., N_c]$. (The $y_n$ and $\hat{y}_n$ values do not necessarily have to be the same.)

Once the array containing the values $\hat{\phi}^+(y_n, c_m)$ is built, it is used to compute the integrals. A first option consists in combining a classic numerical scheme away from the singularity, such as trapezoid rule, with an exact integration of the local expansion in a small neighborhood of the singular point containing a number $d$ of grid segments ($d \approx 5$). In this way we obtain

$$
\hat{\Phi}_k(y_n, t) \approx \sum_{m=1}^{n-d} \hat{\phi}_k^+(y_n, c_m)w_k^+(c_m)e^{-icm_{m}\Delta_m} + \sum_{m=n+d}^{M} \hat{\phi}_k^-(y_n, c_m)w_k^-(c_m)e^{-icm_{m}\Delta_m} + I_d,
$$

as an approximation of (5.8), for instance. In the above expression $\Delta_m$ represents the appropriate weight corresponding to the trapezoid-rule, and $I_d$ the exact integration of the expanded integrand. Depending on the software, it could be more efficient, both in terms of implementation and computation time, to follow a slightly different strategy. If the software of choice is Mathematica, it was found to be very convenient to use the built-in function \texttt{NIntegrate}, which is capable of handling singularities accurately avoiding slow symbolic computations. This provides reasonably fast and accurate computation with the minimum of coding efforts.

5.4 Discussion

We have presented and analyzed by means of rigorous asymptotic methods a new class of exact solutions for linearized perturbations in stratified parallel shear flows. Such solutions generalize a previous exact result [38] to general shear profiles, and, perhaps most notably, include its spatial analog. These results provide substantial physical information on the role of the continuous spectrum in stratified shear flows. In particular, we have shown how the continuous spectrum is connected to a reversible
mechanism of enhancement-by-compression, which naturally converts into damping-by-filamentation after the perturbation structures are overturned by the shear—this is also consistent with the transient nature of non-normal growth. The physical features illustrated through specific examples are robust properties of perturbations contained in the continuous spectrum (i.e. they hold for general shear backgrounds and initial perturbations), as they are a consequence of the mathematical structure of the continuous spectrum solutions.

5.4.1 Future developments

From a broader viewpoint, these results allow to argue that the filamentation observed in wave-induced shear layers could be due essentially to the same mechanism. For this to be the case, it is necessary that the perturbation energy, which starts entirely contained in the discrete spectrum, can “leak” on the continuous spectrum band, as symbolically represented in figure 5.8. A verification of such conjecture and the development of more rigorous mathematical basis are interesting results to pursue in future work.

Another interesting avenue of investigation consists in the search for specific upstream perturbations that give rise to transient non-normal growth, where the perturbations considered so far exhibit pure decay. This possibility has been explored for the case of parallel shears [38], which may provide useful guidelines once again.
Figure 5.8: Sketch of the spectrum excited by an upstream perturbation illustrating the hypothesis of energy leak on the continuous spectrum (which lies in the entire area enclosed between the thick gray curves representing the velocity extrema). The picture is based on a replica of figure 3.3b, which contains the eigenvalue branches (real part) along a wave-induced shear layer. See the referred plot for further details.
Part II

ANOMALOUS DIFFUSIVE REGIMES OF PASSIVE TRACERS IN SHEAR FLOWS
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 [104], see also the recent survey [68] on turbulent mixing). The general advection-diffusion equation is
\[ T_t + \nabla (uT) = D \nabla^2 T \]
where \( T(x,t) \) is the scalar concentration, \( u(x,t) \) is the advecting velocity field which can depend on space and time, and \( D \) is diffusivity of the scalar. The above equation is used to model the evolution of physical quantities such as temperature or concentration of chemical agents dissolved in a fluid—under the assumption that the underlying flow is not affected by \( T \), whereby \( u(x,t) \) is regarded as a prescribed function. Equation (6.1) must be provided with initial data, \( T(x,0) = T_0(x) \), and suitable boundary conditions. A number of factors can characterize the complexity of the problem (e.g., dimensionality, structure of the velocity field, 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 the one considered in the seminal work by Taylor [94]. Taylor was the first to show that, in a laminar pipe flow with radius $r$ and centerline flow speed $V$, the evolution of $T$ is governed by a one-dimensional renormalized diffusion equation for long times, with effective diffusivity

$$D_{\text{eff}} = D \left[ \frac{1}{192} \left( \frac{V}{D} \right)^2 + 1 \right].$$

This formula shows that, if $D \ll Vr$, the effective diffusivity is much larger than the bare molecular diffusivity. This result, often referred as “Taylor diffusion” (or “Taylor–Aris diffusion”, due to the contribution by Aris [7] that came shortly after), allows for a much more concise description of the evolution. Taylor also established that the renormalized 1D-evolution sets in at time scales $t \gg r^2/D$.

Since then, only some attention has been paid to the full evolution from initial data to the long-time limiting behavior. The finite-time features of the problem have been considered by some authors focusing on the identification of transient stages acting on intermediate timescales. Transient dynamics can be physically relevant in many situations. For example, dispersion of pollutants in rivers [104] 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 become the focus of interest. Examples include Spiegel & Zaleski [88] and Doering & Horsthemke [34], these studies recognize that the stability analysis of an advection-diffusion-reaction system builds on the eigenmodes of the advection-diffusion problem.

By using a free-space solution introduced by Lighthill [61], Latini & Bernoff [59] have studied the complete evolution of $\delta$-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 super-diffusion, and Taylor dispersion. The first time scale is well-known to be very dependent on initial conditions, as also Camassa et al. [20] have rigorously shown for pipe flows; the second one is often close to the cross-stream diffusive time $r^2/D$. Since one focus of our investigation is the questioning of $r^2/D$ as the universal timescale that marks the transition into the Taylor regime, we will refer to the timescale in which the homogenized equation becomes a good approximation to the evolution as the “Taylor regime timescale,” to be distinguished from the above diffusive timescale 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 modes [22] (see also [81] for scaling arguments). Camassa et al. [22] 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 & Young [81]. 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 non-periodic problems on intermediate time scales. We remark that this viewpoint is also used by Sukhatme & Pierrehumbert [92], who described the scalar evolution with more complex velocity fields in terms of emerging self-similar eigenmodes.

The goal of this work is to develop a mathematical picture able to explain the above observations in precise mathematical terms, and that can present the different diffusive regimes in a more unified picture. This mathematical picture is centered around the analysis of the spectrum of the advection-diffusion operator. Chapter 7 contains the formulation of the eigenvalue problem, the mathematical theory—in particular the WKBJ analysis, which will be an essential tool in the rest of the study. The rest of the analysis, in chapter 8, is organized in two steps: (i) a detailed study of the spectrum and eigenmodes of the advection-diffusion equation in parallel shear layers; and (ii) a numerical investigation of the connection between the spectrum and the time evolution of initial value problems with strongly multiscale initial data.
Chapter 7

WKBJ ANALYSIS FOR ADVECTION-DIFFUSION PROBLEMS

The mathematical tools necessary for the analysis of passive scalar dispersion in different kinds of shear flows are the focus of this chapter, which is organized as follows. In Section 7.1 the formulation of the eigenvalue problem derived from the advection-diffusion equation is presented. This will lead to a periodic second order non-self-adjoint operator. While the spectral theory for second order self-adjoint periodic equations (Floquet theory) is rather complete [67], 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. [12], and some existence results for complex spectrum have been obtained by Shin [85]). Here we derive simple bounds for the complex spectrum. It is emphasized how the advection-diffusion equation in shear flows leads to a problem possessing a WKBJ structure in the limit of large Peclét number, which is of primary interest in the study of chapter 8. In §7.2 the general WKBJ theory for second order operators is reviewed in a rather non-standard perspective. Emphasis is given to the formulation in the complex plane, which is required in order to set the method in a powerful perspective suitable to handle non-self-adjoint eigenvalue problems. The asymptotic matching technique to find eigenvalues in smooth shear flows is presented in §7.3. In §7.4 are separately examined the particular cases of a “sawtooth” shear flow and circular convective cell,
which require a modified approach.

7.1 The advection-diffusion eigenvalue problem

The advection-diffusion equation, assuming the velocity field to be a parallel shear $u(y)$, is

$$T_t + u(y)T_x = Pe^{-1}\nabla^2 T,$$  \hspace{1cm} (7.1)

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 non-dimensionalization 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 $2\pi$. The Peclét 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 (7.1) is expanded as

$$T(x, y, t) = \int_{-\infty}^{\infty} dk \sum_{n=0}^{\infty} a_n(k) \psi_n(y, k) e^{\omega_n t + ikx},$$  \hspace{1cm} (7.2)

being $\psi_n(y)$ the eigenfunctions basis associated with the wavenumber $k$, and $\omega_n$ the corresponding complex frequency. The freedom in $k$ introduces a second length scale $L_{tracer}$, connected to the initial data on (7.1). Using (7.2) into the evolution equation, and projecting onto the adjoints, the eigenfunctions are found to satisfy

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

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Introducing
\[ \epsilon = 1/(kPe), \quad \lambda = \omega/k + k^2 \epsilon, \]
we finally write the periodic eigenvalue problem in normalized form
\[ \begin{cases} 
\epsilon \psi_{yy} = \left( \lambda + i u(y) \right) \psi, \\
\psi(-\pi) = \psi(\pi), 
\end{cases} \]
(7.3)
for the eigenfunction \( \psi(y) \) and the eigenvalue \( \lambda \).

Notice that when the solution of (7.1) 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 \( \epsilon \) can be regarded as a positive definite quantity.

### 7.1.1 Exact estimates on \( \lambda \)

It is possible to show \textit{a priori} that \( \lambda \) 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
\[ \lambda_R < 0, \quad -1 < \lambda_I < 1. \]
(7.4)

Multiplying both sides of (7.3) by \( \psi^* \), and summing each side of the resulting equation to the adjoint part, is obtained the relation
\[ \left( \psi^* \psi_y + \psi_y^* \psi \right)_y - 2|\psi_y|^2 = 2\epsilon^{-2} \lambda_R |\psi|^2. \]
Integrating over the period $P$ we have

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

which implies the first one of (7.4). If, otherwise, we repeat the procedure subtracting the adjoint part, we obtain

$$
(\psi^* \psi_y - \psi \psi^*_y)_y = 2e^{-2} (\lambda I + u) |\psi|^2,
$$

and integration now yields

$$
\int_P (\lambda I + u)|\psi|^2 \, dy = 0.
$$

Such 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 (7.4) follows.

## 7.2 WKBJ solutions in the complex plane

The concepts we are going to use can be traced back to the earlier studies of the Schrödinger equation of quantum mechanics (see for instance Dunham [36]). Similar ideas have later appeared in fluid mechanics literature, with special attention to the early developments in stability theory, pioneered by Lin [62] and, even earlier, by Heisenberg [46]. Unlike the typical quantum mechanics turning-point problems the present analysis demands additional effort, due to non-self-adjointness of the underlying operator and consequent existence of a complex spectrum. Some credit for complex WKBJ analysis should certainly be attributed to Wasow [101], in particular in connection to the Stokes phenomenon (see discussion below), which is central to this problem.

The WKBJ method is used to find asymptotic solutions to an ordinary differential
equation in the form
\[ \varepsilon \psi_{yy} - q(y, \lambda) \psi = 0, \quad (7.5) \]
for \( \varepsilon \to 0 \). From the above formula it is apparent that WKBJ belongs to the family of singular perturbation methods, since the small asymptotic parameter \( \varepsilon \) multiplies the highest derivative in the problem. Even though the method also applies to higher order equations, our interest here is limited to the second order case. We incorporate a parameter \( \lambda \) from the outset, as eventually we will be interested in solving eigenvalue problems in \( \lambda \) for specific choices of the “potential” \( q(y, \lambda) \):

\[
\begin{cases}
\varepsilon \psi_{yy} - q(y, \lambda) \psi = 0, \\
\psi(a) = \psi(b) = 0,
\end{cases}
\quad (7.6)
\]

The WKBJ method establishes that the \( \varepsilon \to 0 \) limiting solutions of (7.5) are in the form
\[
\phi_{1,2} = q(y; \lambda)^{-1/4} \exp \left( \pm \varepsilon^{-1/2} \int_{y_0}^y q(\zeta; \lambda)^{1/2} d\zeta \right),
\quad (7.7)
\]
which is derived from assuming an asymptotic expansion
\[
\psi \sim \exp \left[ \varepsilon^{-1} \sum_{n=0}^{\infty} \varepsilon^n S_n(y) \right], \quad \varepsilon \to 0,
\]
see, e.g., [13]. Note that so far \( y_0 \) is left unspecified in (7.7). Also the domain of validity of such asymptotic solutions is not specified as yet. The breakdown of (7.7) close to turning-points is a well known fact, moreover WKBJ solutions fail to hold uniformly in a whole annular region looping around a turning-point [101] (Stokes phenomenon). We point out that WKBJ solutions (7.7) have a well-defined meaning only after the domain of definition is specified. In fact, one WKBJ solution can be asymptotic to different exact solutions in different regions of the complex plane. These ideas have been fully
formalized in the work of Wasow [101], which will be summarized in what follows. It will be explained how, in the case of simple turning points, three independent WKBJ solutions are needed in order to have a complete basis of asymptotic solutions around a simple turning point. It could be said that—allowing for a bit of provocation—second-order ODEs possess three independent solutions.

7.2.1 Wasow theorem and connection formulas

The connection formulas used in WKB calculations are here derived following an argument based on a theorem due to Wasow [101]. For conciseness such a result is not reported in its original form and full generality, but it is restricted to the needs of the present discussion.

A few definitions are first required. Let \( h(y) \) be an analytic function with a simple root at \( y = y_0 \), and \( Q(y) = \int_{y_0}^{y} h(\zeta)^{1/2} d\zeta \). Let \( \mathcal{T} \) be a doubly connected open set surrounding \( y_0 \) defined by \( 0 < |Q(y)| \leq K \), for \( K \) small enough to guarantee that no roots of \( h \) are contained in \( \mathcal{T} \). Being \( y_0 \) a simple root, there are three curves \( \mu_k \), with \( k = 1, 2, 3 \), emanating from \( y_0 \) where \( \text{Re}[Q(y)] = 0 \). Hereafter such curves will be referred as Stokes lines. The Stokes lines divide \( \mathcal{T} \) in three open subsets, we denote as \( \mathcal{S}_k \) the one not delimited by \( \mu_k \). The following result can now be stated.

**Theorem 1 (Wasow)** Let \( w_k(y) = h^{-1/4} \exp \left( \epsilon^{-1/2} Q(y) \right) \) for \( k = 1, 2, 3 \), with the square roots determined to be analytic in \( \mathcal{T}/\mu_k \) with negative real part in \( \mathcal{S}_k \). Then the asymptotic relation

\[
    w_k \sim u_k, \quad \epsilon \to 0
\]

is valid in \( \mathcal{T}/\mu_k \), where \( \epsilon u_{kyy} + h(y)u = 0 \).

The situation is sketched in figure 7.1, where the domains of validity of the asymptotic solutions \( w_k \) are represented. Two remarks are now in order.
1. The branch choice assumed in the theorem for the square roots ($\mu_k$ is the branch-cut for $w_k$) implies that $w_k$ is exponentially small in $S_k$ and exponentially large in the other two curvilinear sectors. The Stokes lines mark the transition between the distinct behaviors.

2. If $w_1$, say, is analytically continued from $S_3$ to $S_2$ crossing $\mu_1$ (counter-clockwise) we have $w_1 = w_2$ in $S_2 \cup \mu_1 \cup S_3$, otherwise, we have $w_1 = w_3$ if $w_1$ is analytically continued from $S_2$ to $S_3$ (clockwise).

![Figure 7.1: Domains of validity of the three asymptotic solutions $w_k$.](image)

The $w_k$’s are pairwise linearly independent, hence any two of them can be linearly combined to obtain an asymptotic representation of any solution of (8.6) in the equally labeled sectors and the Stokes line in between. For example, $w_2$ and $w_3$ define a basis for asymptotic solutions in $S_2 \cup \mu_1 \cup S_3$. Observe how the same freedom is not available in $S_1$ since $w_2$ and $w_3$ are not independent therein, indeed they are both exponentially large. An exponentially small solution in $S_1$ can there be represented only by $w_1$ (the
existence of such a solution is implied by Thm 1 itself). It follows that it is possible to establish the following asymptotic equivalence between either one of the $w_k$’s, say again $w_1$ and a linear combination of the other two:

$$w_1 \sim \gamma w_2 + \delta w_3, \quad \epsilon \to 0, \quad y \in S_2 \cup S_3,$$

(7.8)

for some constants $\gamma$ and $\delta$. This fact allows to choose, besides $w_k$, an alternative asymptotic expressions for the exact solution $u_k$. The important difference lies in the fact that the second choice yields an asymptotic solution uniformly valid in $S_1 \cup \mu_3 \cup S_2$.

The constants $\gamma$ and $\delta$ are determined in the following way. Observe first that as $w_3$ is subdominant in $S_3$ and $w_2$ is subdominant in $S_2$, the asymptotic equality (7.8) is held up by a single function in each sector. Hence $\gamma$ and $\delta$ are obtained by matching $w_2$ and $w_3$ with $w_1$ in $S_3$ and $S_2$ independently. Secondly, some ambiguity is still present in the definition of the $w_k$, in fact the branch-choice for the exponential term doesn’t uniquely determine $h^{-1/4}$. Even though this simply consists in fixing a normalization constant, $\gamma$ and $\delta$ depend on such choice. Let the branch of $h^{-1/4}$ be chosen such that $w_1 = w_2$ in $S_3$ and equally determined for $w_3$ in this sector. In moving from a given point $y_A \in S_3$ to a point $y_B \in S_2$ we have to loop around $y_0$ clockwise to avoid crossing $\mu_1$, and counter-clockwise to avoid crossing $\mu_3$. This implies a difference of $\pi/2$ in $\arg(h^{1/4})$ whether it appears in $w_1$ or $w_3$. Therefore, $w_1 = iw_3$ in $S_2$, and we have determined that

$$\gamma = 1, \quad \delta = i.$$

The switch of asymptotic representation is schematically shown in figure 7.2, and this operation is denoted by

$$w_1 \rightarrow w_2 + iw_3$$

(7.9)

in our notation. By the second one of the remarks pointed above, it is possible to
Figure 7.2: In $\mathcal{S}_1 \cup \mu_2 \cup \mathcal{S}_3$ the function $w_1$ can be interchanged with $\gamma w_2 + \delta w_3$, the second one however gives uniform asymptotics in this set.

consider $w_2$ in (7.9) as the analytical continuation of $w_1$ from $\mathcal{S}_3$ through $\mu_1$, and in practice, with slight abuse of notation, we could work with only two fundamental solutions instead of three writing (7.9) as

$$w_1 \rightarrow w_1 + iw_3.$$  

(7.10)

7.3 Computing eigenvalues using WKBJ: asymptotic matching

After the connection formulas have been obtained, we can focus back the attention on the eigenvalue problem (7.6). We assume that the potential well $q$ has the structure

$$q(y, \lambda) = V(y) + \lambda,$$

where $V(y)$ is an analytic function, possessing a critical point at $y = 0$.

If the value of $\lambda$ is close enough to $V(0)$, and the local behavior of $V$ around $y = 0$ is parabolic, two simple turning-points, $y_L$ and $y_R$, exist close to the $y$-origin. Three Stokes lines emanate from each of $y_L$ and $y_R$, and the same number of anti-Stokes lines. We remind that Stokes lines are defined by $\text{Re}[\int_{y_0}^{y} q(\zeta, \lambda)^{1/2}d\zeta] = 0$, while anti-Stokes
lines are defined by the specular condition $\text{Im}[\int_{y_0}^{y} q(\zeta, \lambda)^{1/2} d\zeta] = 0$ with $y_0$ being either $y_L$ or $y_R$. In figure 7.3 is reported a plot of such curves in the complex $y$-plane, which depicts the typical configuration corresponding to turning-points localized near at the critical point of a locally parabolic potential well. (Precisely, this plot is based on the case that will be discussed in § 8.2.2.)

On the Stokes and anti-Stokes lines WKBJ 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 WKBJ solutions $\phi_{1L}, \phi_{2L}, \phi_{1R}$ and $\phi_{2R}$, where the subscript indicates the specific choice $y_0 = y_L$ or $y_0 = y_R$. The sector of definition of both $\phi_{1L}$ and $\phi_{2L}$ is the one contained in between $\mu_{L2}$ and $\mu_{L3}$ (unshaded left region in Fig.7.3). Similarly $\phi_{1R}$ and $\phi_{2R}$ are defined in between $\mu_{R2}$ and $\mu_{R3}$ (unshaded right region in Fig.7.3). Also, the branch choice implies that $\phi_{1L}$ is the exponentially small solution for $y$ moving left along the negative real axis, while $\phi_{2R}$ is small for $y$ moving right along the positive real axis.

As we work under free-space conditions, only the vanishing components of the solution (i.e. $\phi_{1L}$ and $\phi_{2R}$) are present in the far field, the white regions extending indefinitely in figure 7.3. To determine eigenvalues one has to impose matching in the middle region $S$ (shaded region in Fig.7.3) between left- and right-handed solutions, that correspond to $\phi_{1L}$ and $\phi_{2R}$ in the lateral far-field sectors. Moving from the far field into $S$ the two asymptotic solutions $\phi_{1L}$ and $\phi_{2R}$ must be continued inside $S$ by using the connection formulas. In other words, $\phi_{1L}$ and $\phi_{2R}$ must be replaced by different expressions in order to be asymptotic to the same exact solution inside $S$. By following the convention that the four functions $\phi$ are extended inside $S$ by analytic continuation looping counter-clockwise around the turning-points, the connection formulas, as found
Figure 7.3: Stokes (dashed) an anti-Stokes (continuous) lines for turning-points close to the origin. The shaded region is the (open) set $S$.

in the previous section, are

$$\phi_{1L} \rightarrow \phi_{1L} + i\phi_{2L}, \quad (7.11a)$$

$$\phi_{2R} \rightarrow \phi_{2R} + i\phi_{1R}. \quad (7.11b)$$

We remark again that these are analogs of Jefferey’s connection formulas [52, 13], 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.

After using the connection formulas, we can enforce matching inside $S$ and obtain an eigenvalue condition. This can be performed in either a symmetric or anti-symmetric manner

$$\phi_{1L} + i\phi_{2L} = \pm\phi_{2R} \pm i\phi_{1R}. \quad (7.12)$$
For compactness of notation let

\[ Q_L = \epsilon^{-1/2} \int_{y_L}^{y} q(\zeta, \lambda)^{1/2} d\zeta, \quad (7.13) \]

\[ Q_R = \epsilon^{-1/2} \int_{y_R}^{y} q(\zeta, \lambda)^{1/2} d\zeta, \quad (7.14) \]

equation (7.12) (dropping the prefactor \( q^{-1/4} \)) becomes

\[ e^{Q_L} + i e^{Q_L} = \pm e^{-Q_R} \pm i e^{Q_R}, \]

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

\[ e^{Q_{LR} + Q_R} + i e^{-Q_{LR} - Q_R} = \pm e^{-Q_R} \pm i e^{Q_R}, \]

which can be recombined as

\[ e^{Q_R} [e^{Q_{LR}} \mp i] = e^{-Q_R} [-i e^{-Q_{LR}} \mp 1]. \quad (7.15) \]

The last relation can be satisfied if the terms in brackets are equal to zero. After a few straightforward manipulations, the above eigenvalue condition for complex turning-points yields the following implicit relation in the eigenvalues \( \lambda \)

\[ \exp \left( \epsilon^{-1/2} \int_{\gamma} q(\zeta; \lambda)^{1/2} d\zeta \right) = \pm i, \quad (7.16) \]

where \( \gamma \) 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 \( q(\zeta; \lambda)^{1/2} \)). Notice how the above integral condition appears as a natural extension of the well-known result for self-adjoint problems, where the turning-points lie on the real line [13]. Equation (7.16)
can be rewritten as

\begin{equation}
\int_{\gamma} q(\zeta;\lambda)^{1/2} d\zeta = i \epsilon^{1/2} \pi (n + \frac{1}{2}), \quad n = 0, 1, 2... \tag{7.17}
\end{equation}

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

### 7.4 Variants of WKBJ analysis in specific cases

The method just described represents the general way of extracting eigenvalues using WKBJ analysis for analytic potential functions. There are cases of interest which do not satisfy this assumption, but are still amenable of analytical study by using modified approaches. Two particularly significant examples are reported below.

#### 7.4.1 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 (7.3), which now reads as

\begin{equation}
\epsilon \psi_{yy} = (\lambda + i |y|) \psi, \tag{7.18}
\end{equation}

can be solved in the \( \epsilon \to 0 \) limit by a patching method. The starting point is again the assumption of the ansatz (8.7).
**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 \(\psi\) will be in general a linear combination of two independent solutions of (7.18), say \(\psi_1\) and \(\psi_2\). The boundary conditions require the existence of a non trivial solution for the linear system

\[
\begin{align*}
\gamma \psi_1'(0) + \delta \psi_2'(0) &= 0 \\
\gamma \psi_1'(2) + \delta \psi_2'(2) &= 0
\end{align*}
\]

in the symmetric case, or

\[
\begin{align*}
\gamma \psi_1(0) + \delta \psi_2(0) &= 0 \\
\gamma \psi_1(2) + \delta \psi_2(2) &= 0
\end{align*}
\]

in the antisymmetric. Setting the determinant equal to zero we obtain the eigenvalue condition, but before writing it, we make \(\psi_1\) and \(\psi_2\) 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 (7.18) 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 $A_1(z) = Ai(z)$ and $A_2(z) = Ai(\omega z)$, 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

$$A_1'(z_+)A_2'(z_-) = A_1'(z_-)A_2'(z_+), \quad (7.19)$$

$$A_1(z_+)A_2(z_-) = A_1(z_-)A_2(z_+). \quad (7.20)$$

The ansatz for $\lambda$ implies that we assume the form

$$z_+ \sim 2i^{-5/3}\epsilon^{-1/3} \quad (7.21)$$

$$z_- \sim i^{-2/3}(a\epsilon^{p-1/3} + ib\epsilon^{q-1/3}) \quad (7.22)$$

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 $i^\alpha$, we have the constraint $\frac{1}{3} \leq \alpha \leq \frac{4}{3}$.

**Determination of $p$ and $q$**

We first show that assuming either $p < \frac{1}{3}$ or $q < \frac{1}{3}$ (i.e. $z_- \to \infty$), then (7.19) and (7.20) 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 $p = q = \frac{1}{3}$. 

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

\[
\begin{align*}
\frac{A_1(z_+)}{A_2(z_+)} &= \frac{A_1(z_-)}{A_2(z_-)} \\
\frac{A'_1(z_+)}{A'_2(z_+)} &= \frac{A'_1(z_-)}{A'_2(z_-)}.
\end{align*}
\] (7.23) (7.24)

Planning to obtain the $\epsilon \to 0$ 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.

**Antisymmetric case** The leading order behavior of $A_1(\rho i^\alpha)$ and $A_2(\rho i^\alpha)$ as $\rho \to +\infty$ is known to be [2]

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

\[
A_1(\rho i^\alpha) \sim \rho^{-1/4} \exp \left( -\frac{2}{3} \rho^{3/2} i^{3\alpha/2} \right),
\] (7.25)

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

\[
A_2(\rho i^\alpha) \sim \rho^{-1/4} \exp \left( \frac{2}{3} \rho^{3/2} i^{3\alpha/2} \right),
\] (7.26)

where the actual constants which 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 (7.23) follows directly from the above formulas. In fact from (7.21) we are in the case $\alpha = -\frac{5}{3}$, in which both (7.25) and (7.26) are valid. Using (7.21) and developing the ratio we obtain

\[
\frac{A_1(z_+)}{A_2(z_+)} \sim \exp \left( -\frac{8\sqrt{2}}{3} \epsilon^{-1/2} i^{-5/2} \right).
\] (7.27)

For the right-hand side, we notice that (7.22) implies that, if $z_-$ is assumed to go
to infinity as $\epsilon \to 0$, it has to belong to the sector $S$ given as $\frac{\pi}{6} \leq \arg(z_-) \leq \frac{2\pi}{3}$ (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 sub-sectors $S_1$ and $S_2$, defined by $\frac{\pi}{3} < \arg(z_-) \leq \frac{2\pi}{3}$ and $\frac{\pi}{6} \leq \arg(z_-) < \frac{\pi}{3}$. In sector $S_1$, it should be used (7.26) with $\frac{2}{3} < \alpha \leq \frac{4}{3}$, which falls outside the range of validity for that asymptotic expansion. Hence $\alpha$ 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:

- **Sector $S_1$, $\frac{2}{3} < \alpha \leq \frac{4}{3}$:**

  \[ A_{1,2}(\rho i^{\alpha}) \sim \rho^{-1/4} \exp \left( -\frac{2}{5} \rho^{3/2} i^{3\alpha/2} \right). \]

  It follows:

  \[ \frac{A_1(z_-)}{A_2(z_-)} \sim \text{const.}, \quad \epsilon \to 0 \]  

  (7.28)

- **Sector $S_2$, $\frac{1}{3} \leq \alpha < \frac{2}{3}$:**

  \[ A_1(\rho i^{\alpha}) \sim \rho^{-1/4} \exp \left( -\frac{2}{5} \rho^{3/2} i^{3\alpha/2} \right), \]

  \[ A_2(\rho i^{\alpha}) \sim \rho^{-1/4} \exp \left( \frac{2}{5} \rho^{3/2} i^{3\alpha/2} \right). \]

  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 (7.22)

  \[ \frac{A_1(z_-)}{A_2(z_-)} \sim \exp \left( -\frac{4}{3} (a^2 + b^2)^{3/4} \epsilon^{\frac{3\alpha-1}{2}} i^{3\alpha/2} \right), \quad \epsilon \to 0. \]  

  (7.29)
Now it is possible to compare the asymptotics of left- and right-hand side of the eigenvalue condition (7.23). It is almost immediate to realize that no matching is possible. Indeed, from (7.27) it is clear that left-hand side is asymptotically a growing exponential, while neither (7.28) and (7.29) 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 (7.22) this immediately implies \( p \geq \frac{1}{3} \) and \( q \geq \frac{1}{3} \).

**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 \( \rho \), which is [2]

\[
\begin{align*}
\text{for } &\alpha \in (-2, 2) \\
A_1'(\rho i^\alpha) &\sim \rho^{1/4} \exp \left( -\frac{2}{3} \rho^{3/2} i^{3\alpha/2} \right), \\
\text{for } &\alpha \in (-\frac{10}{3}, \frac{2}{3}) \\
A_2'(\rho i^\alpha) &\sim \rho^{1/4} \exp \left( \frac{2}{3} \rho^{3/2} i^{3\alpha/2} \right),
\end{align*}
\]

(7.30) (7.31)

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 (7.24) cannot hold unless \( p \geq \frac{1}{3} \) \( q \geq \frac{1}{3} \).

**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 (7.23) and (7.24) 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 \( A_1(z_-)/A_2(z_-) \to \infty \), 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 \( e^{i\frac{\pi}{3}} \) 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 \( \epsilon \to 0 \), \( O(\exp(-\text{const. } \epsilon^{-\frac{1}{2}})) \), using (7.23) and (7.27) 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 (7.22) is determined, and the remainder for the leading order expression of \( \lambda \) 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 \( \epsilon \), which may be found by using any root-finding numerical algorithm on (7.19) and (7.20). The above scalings results are confirmed by a numerical approach. Moreover an additional behavior at fixed value of \( \epsilon \) merits mention, namely that the imaginary part of the ground-state
eigenvalue vanishes at a critical finite value of \( \epsilon \), indicating non-analytic bifurcations of the eigenvalues. This is in agreement with previous findings by Doering & Horsthemke [34] in the case of a linear-shear channel (mostly equivalent to our “sawtooth.”)

### 7.4.2 Cellular flow

Now we extend the same kind of analysis to a shear flow with closed circular streamlines. The velocity field expressed in tangential and radial components \( u = u_\theta \hat{\theta} + u_r \hat{r} \) is defined as

\[
u_\theta(r) = r \Omega(r), \quad u_r = 0
\]

where \( \Omega \) is an angular velocity. In polar coordinates the advection diffusion equation is

\[
T_t + \Omega(r) T_\theta = \epsilon \left( T_{rr} + \frac{1}{r} T_r + \frac{1}{r^2} T_{\theta\theta} \right).
\]

To illustrate how the approach can be applied to a cellular flow we consider \( \Omega(r) = \Omega_0 - r^2 \). After the separation \( T = e^{\lambda t + i m \theta} \psi(r) \) the eigenvalue problem turns out to be

\[
\epsilon \left( \psi_{rr} + \frac{1}{r} \psi_r - \frac{m^2}{r^2} \psi \right) = (\lambda + i m \Omega) \psi, \quad (7.32)
\]

where for eigenvalues are intended those values of \( \lambda \) that allow for bounded and smooth solutions. The new feature respect to the parallel flow case lies in the singularity at the origin, which is another point beside the TPs where WKB asymptotics break down.

This velocity choice allows for exact solutions, suitable for assessing the accuracy of the forthcoming asymptotic calculation. Solutions of (7.32) are found in terms of generalized \( p^{th} \)-order Laguerre polynomials \( L^\alpha_p \): it is straightforward though somewhat tedious to check (see [60], §4.18) that the analytic solution of eq. (7.32) is given as

\[
\psi(r) = s^\alpha e^{-s^2/2} L^m_p(s^2),
\]

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Figure 7.4: Ground-state mode for the cellular flow ($\epsilon = 10^{-3}$).

with

$$s = e^{-i\pi/8} \left( \frac{m}{\epsilon} \right)^{1/4} r;$$

$$p = \frac{m}{2} + \frac{1}{2} - \frac{\lambda + im\Omega_0}{4} (-im\epsilon)^{-1/2},$$

and the eigenvalues — determined imposing $p$ to be integer, which guarantees $r \to \infty$ decay — are

$$\lambda = im\Omega_0 - \epsilon^{1/2} \sqrt{-im(4n + 2m + 2)}.$$

Away from the origin, setting $r \gg \epsilon^{1/2}$, we have the outer region where WKB can be applied. Neglecting the term $O(r^{-2})$ that would be found to affect only higher order terms if the formal expansion was worked, the transformation $\sqrt{r}\tilde{\psi} = \tilde{\psi}$ reduces (7.32) to

$$\epsilon\ddot{\tilde{\psi}} + (\lambda + im\Omega) \tilde{\psi} = 0,$$

which is now amenable to the standard WKB approximation

$$\tilde{\psi}_{1,2} \sim \phi_{1,2} = h^{-1/2} e^{\pm H}, \quad (7.33)$$
where \( H(r, \lambda) = \epsilon^{-1/2} \int_{r_0}^r h(s) \, ds \) with \( h(r, \lambda) = \sqrt{\lambda + i m \Omega(s)} \). The choice of the correct linear combination of \( \phi_1 \) and \( \phi_2 \) is resolved observing that only \( \phi_2 \) can be an asymptotic approximation of a bounded solution; in the region at the right of \( r_0 \) represented by the shaded sector in Fig.7.5 the solution up to an arbitrary constant is then \( \phi_2 \). Following the same argument of §7.2 we employ the connection formula \( \phi_2 \longrightarrow \phi_2 + i \phi_1 \) in order to represent the same solution in the region between \( r_0 \) and the origin (blank sector in Fig.7.5), we write

\[
\sqrt{r} \psi \sim \phi_1 + i \phi_2. 
\] (7.34)

By perturbing \( H(r, \lambda) \) about \( r = 0 \) we have a small-argument expansion for the above formula

\[
\sqrt{r} \psi \sim \exp \left( H(0, \lambda) - \epsilon^{-1/2} h_0 r \right) + i \exp \left( -H(0, \lambda) + \epsilon^{-1/2} h_0 r \right)
\] (7.35)

Around the origin, for \( r \ll 1 \), we have a local approximation obtained by the inner rescaling \( r' = r/\epsilon^{1/2} \), which yields a Bessel equation (dropping now the primes)

\[
\frac{\partial^2 \psi}{\partial r'^2} + \frac{1}{r'} \frac{\partial \psi}{\partial r'} + \left( -\lambda - i m \Omega_0 - \frac{m^2}{r'^2} \right) \psi = 0.
\]
The local solution given in terms of Bessel function of the first kind [2] is therefore

\[ \psi(r) \sim J_m(\epsilon^{-1/2}r\sqrt{-\lambda - im\Omega_0}), \quad r \ll 1 \]

and the other independent solution of the Bessel equation is rejected being this the only non-singular choice at \( r = 0 \). Using the asymptotic representation of \( J_m \)

\[ J_m(x) \sim \frac{2}{\pi \sqrt{x}} \cos \left( x - \frac{m\pi}{2} - \frac{\pi}{4} \right), \quad |x| \gg 1 \]

we obtain a large-argument expansion of the inner solution

\[ \sqrt{r}\psi \sim \exp \left( \epsilon^{-1/2}r\text{i}h_0 - \frac{m\pi}{2} - \frac{\pi}{4} \right) + \exp \left( -\epsilon^{-1/2}r\text{i}h_0 + \frac{m\pi}{2} + \frac{\pi}{4} \right). \quad (7.36) \]

Outer and inner solutions overlap in the region \( \epsilon^{1/2} \ll r \ll 1 \); matching here we obtain an eigenvalue condition. The two solutions (7.35) and (7.36) can be checked to be linearly dependent, i.e. to match, provided

\[ i \exp (2H(0, \lambda)) = \exp (im\pi + i\pi). \]

It follows immediately the eigenvalue condition

\[ \int_{r_0}^{0} \sqrt{\lambda_n + im\Omega(s)} \text{d}s = i\epsilon^{1/2} \left( m\frac{\pi}{2} + n\pi + \frac{\pi}{4} \right), \]

for \( n = 0, 1, 2, \ldots \) where the integral can be evaluated using straightforward residue-calculation methods. We finally obtain, quite remarkably, the exact result

\[ \lambda = -im\Omega_0 - \epsilon^{1/2}\sqrt{-im}(4n + 2m + 2). \]
Chapter 8

SORTING OF EIGENMODES AT INTERMEDIATE TIME SCALES

The time evolution of a passive scalar advected by parallel shear flows is studied for a class of rapidly varying initial data. As mentioned in the introduction (chapter 6), it is well established that the long-time evolution of the tracer concentration is governed by G.I. Taylor’s asymptotic theory of dispersion. In contrast, we focus here on the evolution of the tracer at intermediate time scales.

8.1 Outline

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 non dimensional 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 $kPe$ is derived for the short scale periodic structure of the scalar’s initial data, for both exactly solvable cases and in general with WKBJ analysis. We show that the sawtooth flow 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 also 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 flow’s interior. A WKBJ study of the latter modes provides a longer intermediate time evolution. When large scale initial data components are present, the transient regime of the WKBJ (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.

This chapter is organized as follows. We start in §8.2 by considering the eigenvalue problem introduced in §7.1, and we characterize the ordering of modes in three classes depending on the interplay of advection with diffusion dictated by the limits $\epsilon \to \infty$ and $\epsilon \to 0$, where $\epsilon = 1/(kPe)$. The limit $\epsilon \to 0$ is further classified into two categories depending on the relative ordering with respect to the balance $k = O(Pe^\alpha)$ where the exponent $\alpha$ is shown to depend on the smoothness properties of the velocity profile. In the first limit ($\epsilon \to \infty$) a straightforward regular perturbation expansion suffices to compute the spectrum, spanning the Taylor regime. In the second limit ($\epsilon \to 0$), for the simplest cases such as piecewise linear shear layers, the analysis can be worked using exact techniques (presented in §7.4.1), while for more general cases we use WKBJ asymptotics. 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 like $\epsilon^{-\frac{1}{3}}$ as $\epsilon \to 0$. In contrast, we establish the different scalings of $\epsilon^{-\frac{1}{4}}$ and $\epsilon^{-\frac{1}{2}}$ for the spatial internal layers and their decay rates, respectively, for generic locally quadratic shear flows.

In Section 8.3 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 multi-scale initial data. In particular, the theory identifies new intermediate time scales, which are missed by classical moments 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 $r^2/D$.

8.2 Three classes of modes

The problem (7.3) can be studied in the two possible asymptotic limits $\epsilon \to 0$ and $\epsilon \to \infty$. Thinking in terms of $Pe$ large but fixed, this represents a subdivision of the modes into an high- and a low-wavenumber category with qualitatively different properties. It is expected to find, for $k$ small enough, a class of modes that at leading order behaves in agreement with Taylor renormalized-diffusivity theory, and that belongs to the realm of homogenization theory. Within the solutions of (7.3) in the $\epsilon \to \infty$ limit will be found a class referred as Taylor-modes. In the opposite limit (as we shall see later), the problem otherwise acquires a WKBJ structure, in this case we shall use the term WKBJ- or anomalous-modes. We stress that the latter class of modes is more correctly to be considered as an intermediate-asymptotic category. Indeed, letting $k \to \infty$, diffusivity will, at some point, eventually dominate over the eigenvalue $\lambda$. This regime will discussed as the pure-diffusive-modes.
8.2.1 The limit $\epsilon \to \infty$: Taylor modes

In such limit, if the following expansions in $\epsilon$ are assumed

\[ \psi_n = \sum_{j=0}^{+\infty} \epsilon^{-j}\psi_{nj}, \quad (8.1) \]
\[ \lambda_n = \sum_{j=0}^{+\infty} \epsilon^{-j+1}\lambda_{nj}. \quad (8.2) \]

then a regular perturbation problem is found. The use of the above expansion inside the eigenvalue problem (7.3) leads to a classical recursive system of equations

\[ O(\epsilon) : \mathcal{L}[\lambda_{n0}]\psi_{n0} = 0, \]
\[ O(1) : \mathcal{L}[\lambda_{n0}]\psi_{n1} = (\lambda_{n1} + iu(y))\psi_{n0}, \]
\[ : \]
\[ O(\epsilon^{1-m}) : \mathcal{L}[\lambda_{n0}]\psi_{nm} = (\lambda_{n1} + iu(y))\psi_{nm-1} + \sum_{p=1}^{m-1} \lambda_{np+1}\psi_{nm-p-1}. \]

where $\mathcal{L}[\lambda_n] = \frac{d^2}{dy^2} - \lambda_n$. The same recursive problem was also derived by Mercer & Roberts [72], 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

\[ \psi_{n0} = \cos ny/\sqrt{\pi}, \quad \lambda_{n0} = -n^2, \quad (n > 0) \]
\[ = 1/\sqrt{2\pi}, \quad \lambda_{n0} = 0, \quad (n = 0) \quad (8.3) \]

for symmetric modes, and

\[ \psi_{n0} = \sin ny/\sqrt{\pi}, \quad \lambda_{n0} = -\left(\frac{n+1}{2}\right)^2, (n \geq 0) \quad (8.4) \]
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 non trivial regularly-diffusive scaling.

 Corrections to the eigenvalue are gives 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 \( \lambda_{n1} \) which 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 \( D_{\text{eff}} = \frac{1}{2} U^2 L^2_{\text{vel}} / D \). 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 \( \epsilon \to \infty \) eigenvalues are given by

\[
\lambda_n \sim \begin{cases} 
-\epsilon n^2 + O(\epsilon^{-1}), & n > 0 \\
-\frac{1}{2} \epsilon^{-1} + O(\epsilon^{-2}), & n = 0
\end{cases}
\]  
          (8.5)

up to the first non trivial order.

8.2.2 The limit \( \epsilon \to 0 \): anomalous modes

As \( \epsilon \to 0 \) 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. [22]. We employ a different approach from the regular perturbation expansion adopted for the Taylor modes. Asymptotics are obtained via WKBJ method. A first time, this is done generalizing the classical matched-asymptotics calculation for real, self-adjoint operators (in the classical literature often referred as the two-turning-points problem, see for instance Bender & Orszag [13]). Here, however, the non-self-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.

**Exactly solvable linear case**

The first exactly solvable special case consists in a non-analytic “sawtooth” shear profile (with full details reported in § 7.4.1). Eigenfunctions in this case are constructed using piecewise patched Airy functions, and eigenvalues correspond to zeros of certain combinations of these functions which 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 & Gilbert [28] for a linear-shear channel with homogeneous Dirichlet boundary conditions for the scalar. We emphasize that this scaling differs 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 Section 8.1 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 [22]. However, as also shown in the Appendix 7.4.1, the eigenfunctions localize to a thinner region that scales like $O(\epsilon^{1/3})$ as opposed to $O(\epsilon^{1/4})$.
for the analytic case, confirming previous numerical findings in [22] (this comparison is depicted in Figure 8.1, 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 non-slip flat wall will localize as (weakly non-parallel) 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 Figure 8.2, following the asymptotic treatment below.

**Exactly solvable cosine-shear**

Our second example of an exactly solvable case is $u(y) = \cos y$. The eigenvalue problem (7.3) in this case reduces to the complex Mathieu equation

$$
\epsilon \psi_{yy} = (\lambda + i \cos y) \psi, \tag{8.6}
$$

whose eigenfunctions can be written as

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

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

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**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 $\lambda$ in the form

$$\lambda \sim a \epsilon^p + i(b \epsilon^q - 1), \text{ as } \epsilon \to 0.$$  \hspace{1cm} (8.7)

In our derivation we use a free-space approximation: since we are interested in spatially-localized eigenmodes, 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.

**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 (8.7), as $\epsilon \to 0$ 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.7.3). The expression (7.17) which determines the WKBJ eigenvalues is not particularly transparent, and still requires numerical tools in order to extract the eigenvalues $\lambda_{\text{WKB}}$. In order to make such expression more amenable of direct analysis one can perform a Taylor expansion of $q(\zeta; \lambda_{\text{WKB}})$, which yields an explicitly integrable form after truncation. Such possibility will not be pursued here, but in § 8.2.2 it will be related to the result obtained therein. We observe instead that condition (7.17), even as it stands, unveils the scaling exponents $p$ and $q$ in (8.7). Both the integrand and the measure of the integration path $\gamma$ are in fact $O(\sqrt{\lambda + i})$, that gives $O(\epsilon^{-1/2}(\lambda + i)) = 1$, and it follows $p = q = 1/2$. 

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\begin{verbatim}
\begin{tabular}{cccc}
\hline
 & $-\lambda_{\text{WKB}}$ (err %) & $-\lambda_H$ (err %) & $-\lambda_{\text{Exact}}$
\hline
$\epsilon = 10^{-1}$ & \\
$n = 0$ & .15496 + .84185i (2) & .15811 + .84189i (4) & .15173 + .84175i \\
$n = 2$ & .70881 + .20448i (2) & .79057 + .20943i (9) & .72412 + .20884i \\
$\epsilon = 10^{-2}$ & \\
$n = 0$ & .04969 + .94999i (.6) & .05000 + .95000i (1.2) & .04937 + .94999i \\
$n = 2$ & .24207 + .74987i (.1) & .25000 + .75000i (3) & .24174 + .74985i \\
$\epsilon = 10^{-3}$ & \\
$n = 0$ & .01578 + .98419i (.2) & .01581 + .98419i (.4) & .01575 + .98419i \\
$n = 2$ & .07827 + .92094i (.04) & .07906 + .92094i (1) & .07824 + .92094i \\
\hline
\end{tabular}

Table 8.1: Approximate and exact eigenvalues, with percentage error on the quantity \( \lambda + i \).
\end{verbatim}

**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 Bender & Orszag [13], that 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 doesn’t suffer of the latter problem and has the value of giving a simple explicit expression for the eigenvalues.

As \( \epsilon \to 0 \) 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

\[
\varphi'' + \left( \nu + \frac{1}{2} - \frac{1}{4} z^2 \right) \varphi = 0, \tag{8.8}
\]
Figure 8.1: 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).

as

$$\varphi = \text{He}_\nu(\pm z/\sqrt{2})e^{-z^2/4}. \quad (8.9)$$

$\text{He}_\nu$ represents the Hermite function of (arbitrary and complex) order $\nu$ (see [60] §10.2). This is exactly the equation one would find expanding (8.6) up to second order about $y = 0$ and applying the transformations

$$\epsilon^{1/4}z = 2^{1/4}e^{-i\pi/8}y, \quad (8.10)$$

$$\nu = \frac{1}{\sqrt{2}}(\lambda + i)e^{-1/2}e^{i\pi/4} - \frac{1}{2}. \quad (8.11)$$

We essentially can view (8.6) as a perturbation problem regularized by the variable rescaling $\epsilon^{-1/4}y$ for $|y| \ll 1$, with leading-order solutions easily constructed from (8.9).

Such solutions can eventually be matched with outer WKBJ solutions to construct global approximants. However, the approximate eigenvalues $\lambda_H$ are determined at the
level of the inner problem only, imposing asymptotic decay. Hence, the eigenvalues are just related to those of the Hermite equation (8.8) through the transformation (8.11). Since the eigenvalues $\nu$ are determined by the condition that $\psi(y)$ be bounded for $|e^{-1/2}y| \to \infty$ along the real axes, one has to account for the phase shift involved in the coordinate transformation (8.10), and to understand the eigenvalues of (8.8) as those values that allow $\varphi$ to vanish for $|z| \to \infty$ 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 $\nu = 0, 1, 2..., \text{it is then elementary to verify that}$

$$\lambda_H = -i - e^{1/2}(1 - i) \left( n + \frac{1}{2} \right), \quad n = 0, 1, 2... .$$

We point out that one would obtain the same result expanding up to second order the integrand in (7.17) 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.

**Comparison** A comparison of the two approaches described above is given in Table 8.1. Generally we obtain good accuracy even for moderately small $\epsilon$, bare WKBJ being always more accurate than the uniform approximation. This results, perhaps unexpected, is 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 $\epsilon$ fixed, decreasing for $\lambda_{WKB}$ and increasing for $\lambda_H$, 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.

**Poiseuille flow: 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, 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 Figure 8.2, generated by a numerical simulation (details of the algorithm are described below in section 8.3) of the passive scalar evolution initially concentrated in a thin strip \((y\text{-independent})\) in an effectively infinite long channel are advected by the flow \( u(y) = 1 - 4(y - 1/2)^2 \), 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 (7.3) 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 figure 8.3, 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.

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Figure 8.2: Snapshots of the time evolution governed by (7.1) with $u(y) = 1 - 4(y-1/2)^2$ and $Pe = 10^3$, from the initial condition $T_0(x, y) = \exp\left(-\left(x - \frac{L_x}{2}\right)^2/\lambda_x^2\right)$, with $\lambda_x = 10^{-3/2}L_x$, and horizontal Fourier period $L_x = 20\pi$, with $n_x = 1024$ and $n_y = 128$ respectively for horizontal and vertical Fourier modes. Snapshots are taken at $t = 0, 7, 16, 27$ from top to bottom. 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).

When such non-trivial balance is achieved the chevron-like 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 non-zero.

In figure 8.4 the position of the tracer distribution peak near the wall is shown for the simulation depicted in figure 8.2, 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
Figure 8.3: 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.

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

8.2.3 The limit $\epsilon \to 0$, $k \gg Pe^{1/3}$: 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 ($Pe^{-1} k^2$) can overcome anomalous diffusion ($k\lambda$) over the whole $k$-spectrum, including Taylor scales. The threshold between WKBJ and pure-diffusive (PD) modes is simply found comparing the timescale $Pe^{1/2} k^{-1/2}$ from the previous section with the streamwise diffusion scale $Pe k^{-2}$. Equating the two characteristic times we have

$$k\lambda_R \sim Pe^{-1} k^2 \quad \Rightarrow \quad k = O(Pe^{1/3}),$$
implying that the condition for pure-diffusive modes is indeed $\epsilon \to 0$ with $k \gg Pe^{1/3}$.

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

### 8.2.4 Poiseuille flow: global view of the spectrum

In order to conclude the analysis we present a summarising comparison between the exact eigenvalues for Poiseuille, cosine and sawtooth flows. Such comparison is reported in figure 8.5. The eigenvalues are computed numerically with high accuracy by using the special functions that pertain to each case, i.e., Hermite (or, equivalently, Parabolic cylinder), Mathieu and Airy functions respectively. The procedure consists of using a root-finding routine on the determinant that arises from enforcing boundary conditions, as illustrated in §7.4.1 for the sawtooth case.
Figure 8.5: Exact eigenvalues for plane Poiseuille flow, cosine flow and sawtooth flow versus wavenumber $k$, for $Pe = 1000$. Top panels: eigenvalue corresponding to the first centerline mode for Poiseuille flow and first mode for cosine flow. Bottom panels: eigenvalue corresponding to the first boundary mode for Poiseuille flow and first mode for sawtooth flow.

The main purpose of the plots is to show how the passive scalar spectrum in cosine and sawtooth flows provide accurate approximations for the full Poiseuille-flow spectrum in the high-wavenumber range. The agreement is due to the localizations of the eigenfunctions, near the flow centerline and boundaries respectively, for short enough wavelengths (i.e., in the WKBJ range). At low wavenumbers the passive scalar falls in the Taylor regime, and the support of the eigenfunction spans the entire flow cross-section. In such conditions the eigenvalues are affected by the global structure of the advecting flow and hence separate. Non-analytic bifurcation, occurring near the transition between the WKBJ and Taylor regimes, are clearly observable in the branches corresponding to the cosine and sawtooth flows, consistently with the remark made in the closing of §7.4.1. Even though the Poiseuille-flow eigenvalues appear to depend
Figure 8.6: $x$-location of the peak of $T$ along two one-dimensional longitudinal slices taken at the centerline and at the boundary of the channel. The numerical simulation is identical to the one reported in figure 8.2, except for a much larger extension of the domain in $x$, which allows for a much longer time before the boundary conditions in $x$ play any role.

smoothly on $k$, the transition that separates the two regimes is markedly sharp. Such sharpness suggests a corresponding fast rearrangement of the eigenmodes structure.

It is interesting to notice that the time evolution of initial value problems bears a signature of the last feature. Figure 8.6 shows further data obtained from numerical simulations of passive scalar evolution in Poiseuille flow. Using the $x$-location of the peak of the spatial distribution of the passive scalar, the picture shows that the transition between short- and long-time evolution is associated with a somehow abrupt change in the spatial distribution, as evidenced by the “kink” occurring at $t = 140$.

### 8.3 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 non-dimensional advection-diffusion equation (7.1), employing the same numerical scheme as [22].
is a pseudo-spectral solver based on Fourier modes in both $x$ and $y$, with an implicit-explicit third-order Runge-Kutta [87] 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 single-scale initial data and then examine non-periodic (longitudinal) evolutions using a period much larger than the horizontal extent of the initial data.

### 8.3.1 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 $\epsilon$ 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 $\gamma$ would be the constant in the exponent.

First we observe in Fig.8.7 some snapshots of the time evolution when the wavenumber is chosen to have $\epsilon$ 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
Figure 8.7: 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 $tPe^{-1/2}k^{1/2} = 0, .032, .095, 1.89$. While this is a single-mode computation in the streamwise direction, the number of Fourier modes used in the cross-flow direction is $ny=256$.

by Rhines & Young [81]. Such process terminates when fluctuations are completely suppressed by shear, after which two long lived, “chevron”-shaped structures localize in thin layers around the shear-free regions. At this stage the decay rate settles on a constant value.

The picture is analogous to the one considered in [22] 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 Shaw et al. 2007 [84]). 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 [84, 100], while generically of order $O(\epsilon^{3/4})$, 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. 8.8 is the opposite limit of $\epsilon$ large, the distribution sets on a Taylor mode with weak dependence from $y$, which is still visible (right picture) because $\epsilon$ is only moderately large.

The decay rate $\gamma$ is shown in Fig.8.9 and 8.10 as obtained from numerical simulations. These two figures report the same data under different rescaling, to emphasize the $\epsilon$ dependence in the behavior. Also, in each figure a reference horizontal line marks the asymptotic decay rates of the WKBJ and Taylor regimes respectively, obtained from the real part of the ground-state eigenvalue given by (8.12) and (8.5). 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 $\gamma$ 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 non-orthogonal ground-state modes, with conjugate eigenvalues corresponding to right- and left-traveling chevron-structures. As long
Figure 8.9: Decay rates from numerical simulations as a function of time for different values of $\epsilon$, obtained setting $Pe = 1000$ and $k = 10^{-p}$ ($p = 0 : 1 : 5$). Axis are rescaled on WKBJ timescale 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.

As $\epsilon$ is small, the two trains of chevrons are each localized in the respective shear-free regions, this 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 non-orthogonality produces oscillations in the decay rate (essentially a constructive-destructive interference depending on the alignment of the two wave trains). The inset in Figure 8.9 shows the exact reconstruction of $\gamma$ using the two Mathieu ground-state functions, confirming this assertion.

The three regimes of modes are represented collectively in Fig.8.11. This figure shows a time-averaged value of $\gamma$ 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
8.3.2 Multi-scale initial data

In the previous section we have seen how streamwise variations of different scales behave under shear-distortion. The homogenization 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

\[ T_0 = (A \sin kx + B)e^{-x^2/\ell^2}, \]  

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 $\ell_x$. We shall keep constant $k$ and $\ell_x$, and to observe enough scale separation the latter are chosen such as $k Pe \ll 1$ and $Pe/\ell_x \gg 1$. In the following we present four simulations, where all parameters are listed in Table 8.2. Visualizations of the passive scalar fields at different times are reported in Figs. 8.12 to 8.15.

$$
\begin{array}{ccc}
\text{Run} & A & B \\
1 & 1 & 1 \\
2 & 0 & 1 \\
3 & 1 & 0 \\
4 & 1 & 0.001 \\
\end{array}
$$

Table 8.2: Parameters used in numerical simulations. For all of them $k = 1$, $\ell_x = 800$ and $Pe = 50$; the number of (de-aliased) Fourier modes used is $nx=12288$ $ny=64$. The fundamental wavenumbers are $k_{x0} = .001$, $k_{y0} = 1$. The simulations are periodic in $x$ with a domain large enough to mimic an unbounded domain on the timescale of the simulations.

The general physical picture that emerges is as follows. At early times, the high

![Figure 8.11: Averaged decay-rate (see text) versus $k$ from numerical simulations. The lines represents the three asymptotic behaviors of $k\Re[\lambda_0]$, including also three simulations from the pure diffusive regime. Results are for $Pe = 1000$.](image)
frequency components of the initial condition govern the main features of evolution, similar to the $x$-periodic problem discussed in the previous section (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-over” time – corresponds to the time when evolution starts to be governed by the homogenized equation (the definition of Taylor timescale used in this paper), and can be different from the non-dimensional cross-flow diffusive time scale, $\tau_D = Pe$.

From a spectral perspective the decay time of the high-frequency spectral bands is estimated by our WKBJ analysis to be $k^{-1/2}Pe^{1/2}$. While this timescale is in general shorter than $\tau_D$ (for large $Pe$), the initial data can be such that the relative energy of the high vs. low frequency bands (e.g., set by the parameters $A$ and $B$ in (8.13)) can make the WKBJ modes observable well beyond $\tau_D$. Further, these differences can be seen by comparing the evolution of moments vs. norms, as we show below.

Looking at the snapshots for Run 1 one can see that by $t = 100$ chevron-like structures are completely depleted. We inquire whether this major structural “cross-over” is a benchmark for the transition to the Taylor regime. Fig.8.17 (top panel) depicts the cross-over 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 non-orthogonality of anomalous modes as discussed in the previous section.

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.8.16 the variance-gap $\tilde{\sigma}(t) := \sigma_T(t) - \sigma(t)$, where $\sigma$ is the variance in
$x$ of the distribution integrated in $y$, and $\sigma_T = 2\pi Pe t$ is the theoretical law for a Gaussian distribution evolving according to Taylor-renormalized pure diffusion. This onset is clearly seen in Fig.8.16. 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 cross-over transition has occurred earlier ($t \approx 10$) than $\tau_D$, which at $Pe = 50$ 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 $\gamma$ (reported in Fig.8.17 (bottom)) settles on a constant value (predictable from WKBJ eigenvalues as shown previously), and the cross-over 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 cross-over 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.8.15).

The difference that stands between the transition at time $\tau_D$ and the smearing out of fast scales is further illustrated by looking at Run 2. Even at large scales, hence at low wavenumbers, 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. Cross-stream diffusion sets this weak variation to a small amplitude $O((Pe \ell_x)^{-1})$ (as given above in the analysis of Taylor modes) once a time scale $O(Pe)$ 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.
Figure 8.12: Snapshots showing the distribution of the passive scalar for Run 1. Time instants are $t = 0, 5, 15, 100$ fro left to right. Only a portion of the domain is shown. Colorbar as in figure 8.2, but ranging from $-1$ to $1$. 

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Figure 8.13: Same as Figure 8.12 for Run 2
Figure 8.14: Same as Figure 8.12 for Run 3
Figure 8.15: Same as Figure 8.12 for Run 4
Figure 8.16: Gap of variance $\bar{\sigma}$ versus time, all distributions are normalized to unitary mass. The curves level off after the time scale $\tau_D$. 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.

Figure 8.17: Time evolution of $L_2$ norm (left) and decay rate (right). Run 2 is not reported in the bottom picture because it would be too low to be visible.
8.4 Concluding remarks

A number of authors [94, 81, 22, 20, 59] have addressed the problem of passive scalar diffusion under simple flow conditions, and non-trivial 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 formulation 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 WKBJ asymptotic analysis provides the longest lived anomalous modes, which persists well beyond the wall boundary layer modes in the limit \( \epsilon \to 0 \).

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 \( k \ll Pe^{-1} \) range. The modes inside the range \( k \gg Pe^{-1} \) characterize the structure of the solution in the super-Gaussian anomalous diffusive regime described, for instance, in the work by Latini & 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 $k_{x0} = 2\pi/L_x \ll 1/Pe$ in order to observe the Taylor regime. A smaller domain, with lower resolution in the wavenumber domain, leads to a cut-off of the Taylor modes, limiting the possible observable regimes up to the “anomalous diffusion” stage. By adjusting the initial relative energy in the bands we demonstrated how the WKBJ may in principle be extended well beyond the classical cross-stream-diffusion timescale $r^2/D$ (or $\tau_D$ in non-dimensional 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.
Part III

NUMERICAL SIMULATIONS OF DENSE-CORE VORTEX RINGS IN A SHARPLY STRATIFIED ENVIRONMENT
Chapter 9

DENSE-CORE VORTEX RINGS IN A SHARPLY STRATIFIED ENVIRONMENT

In this last part of my dissertation it is reported my contribution to the project “Vortex rings dynamics in presence of stratification” currently being pursued at the UNC Fluid Lab. Aim of this project is to isolate essential elements of mixing, trapping, and escape through stratified fluid by focusing on the specific case of dense-core vortex rings settling in sharply stratified miscible ambient fluids for near two-layer configurations. The core of the vortex rings is made of fluid which has density higher than both the top and bottom layers of the ambient fluid, and is fully miscible in both layers. This setup ensures a rich phenomenology including, in particular, a critical (bifurcation) phenomenon which distinguishes long-time behavior of the falling vortex ring in either being fully trapped in the ambient density layer, or continuing through the layer in its downward motion.

My work consists in performing 3D direct simulations supporting the lab experiments conducted by R. Camassa, S. Khatri, R. McLaughlin and K. Mertens, assisted by the undergraduate students D. Nenon and C. Smith. The numerical package VARDEN [6] is used for the simulations. As will be illustrated next, this task presents serious challenges, not limited to the considerable computational size of the problem. In fact, the experimental set up is not reproducible in its entirety, and several efforts go into designing a simplified set up that neglects experimental details (the impact on the free
surface and the following formation process, see discussion in §9.4.2) and yet is able to capture the relevant dynamics. Several significant results have been obtained, which will be presented in this report. However, the study is still open to improvement under several technical aspects and can be completed by collecting further data.

9.1 Introduction

Vertical density stratifications are prevalent in both the atmosphere and the ocean. This background stratification strongly influences the mixing and dispersion properties of fluid and particles passing through them [86, 93]. In some instances this can cause the trapping of particulate matter for long periods of time at locations where they alone are not neutrally buoyant. The recent oil spill in the gulf provides one such example demonstrating subsurface plumes, initially much less dense than sea water, trapping for months several hundred meters below the surface. Another example is the thin layer formation of marine snow aggregates, particles composed of organic and inorganic matter, which has a significant role in the marine carbon cycle [66, 5].

All of these applications involve the dynamics of fluids dragged either by solid particles or self advected in the form of vortices through different density ambient fluids. Much insight can be gained by studying the simplified setup of a single particle or vortex ring dynamics. Recent experimental and theoretical progress has been made on this problem for the case of a single sphere falling through sharp stratification at both moderate Reynolds numbers (300) [89, 1], and low Reynolds numbers (0.001) [18, 17]. In particular, at moderate Reynolds, Abaid et al. [1] demonstrated experimentally that a dense falling sphere could in fact reverse direction and rise on a transient timescale as a plume of light fluid carried by the sphere detached. Further, at low Reynolds numbers, Camassa et al., in the series of papers referenced above, demonstrated both experimentally and theoretically that the falling sphere could undershoot the terminal velocity of the bottom layer, with theory providing fully quantified predictions of the
sphere and fluid dynamics for the entire evolution.

Considerably less is known about miscible dense vortex rings falling through stratified fluids. In homogeneous ambient fluids, when a dense fluid droplet falls under the influence of gravity into a bath of a lighter miscible fluid, a vortex ring is formed and can remain stable to a fairly large penetration depth [27, 10]. The focus of the present study concerns behavior arising from the addition of an ambient sharp stratification. If this vortex ring, in the course of settling, encounters a sharp density ambient fluid transition before reaching its destabilization length scale, the interaction can be nontrivial and potentially lead to the total entrapment of the vortex fluid within this density transition layer. This process is exemplified experimentally in figure 9.1, where a sequence of snapshots of a saltwater vortex ring is settling in a salt stratified environment. Two different outcomes are demonstrated: (1) the vortex ring penetrates below the density transition layer and then rebounds upward settling at the interface between the two layers, (2) the vortex ring continues to settle into the lower layer after penetration and eventually releases the entrained fluid well within the lower layer. This critical phenomena are the focus of this study.

Starting from the seminal work by J.J. Thompson et al. [95], many studies have looked at single and two fluid experiments in this setting. For example, experimental reports concerning the low Reynolds number limit can be found in [55], and examples at moderate Reynolds number can be found in [27, 10, 70]. For the single fluid system much work has also been done in modeling vortex ring dynamics and instabilities ([4]-[71] give a thorough but no way complete list of commonly cited papers). Stratified two fluid problems, where the droplet and top layer density are equal and placed above a sharp stratification, have also been looked at both experimentally [63, 32], and numerically [90].

With the advancement of computational power over recent decades more sophisti-
Figure 9.1: Time snapshots taken from two experiments showing two qualitatively different outcomes: vortex bouncing on the density transition (top), and vortex penetrating trough (bottom). Read discussion in section 9.2.1. The dotted lines reference the location of the density transition, notice that such line is close to the upper margin of the frames in the bottom snapshots. (Experiments by R. Camassa, S. Khatri, R. McLaughlin, K. Mertens, D. Nenon and C. Smith.)

cated methods have been implored to delve into the rich and complicated behavior of the vortex ring problem through direct simulations. In the 1980’s, with computational power still somewhat limited, most work was done in two-dimensions, and with strongly simplified ansatz, boundary integral methods were most commonly used [79, 105]. Coming into the 1990’s more advanced simulations began to appear including vortex sheet methods [78, 64, 39] and viscous dominated axisymmetric Navier-Stokes solvers [69]. In the last decade however, access to more realistic three-dimensional computations have started to become available [90] for the first time allowing deeper probing into these complicated dynamics, those restricted to the case involving a two-layer ambient with vortex ring density matched to that of the top layer. The present study adds the new element of an arbitrary vortex ring density which is different from (denser than) all ambient fluids. This is carried out comparing fully three-dimensional variable density Navier-Stokes simulations to experiments for the case of fully miscible three density systems at moderate Reynolds numbers (of order $10^2$).
This setup poses a challenging task for direct numerical simulations. The numerical solver must be capable of solving the three dimensional, varying density, incompressible Navier-Stokes equations, and of efficiently resolving the fine structures (filamentation) that result from the dynamics of the interacting varying-density fluids. In this respect, note that even in homogeneous ambient fluid, the fluid entrainment that follows vortex ring dynamics poses significant difficulties because of fine scaled structures that must be resolved [39, 90, 35]. Ultimately, diffusion of the stratifying agent will set a cut-off for small-scale filamentation, and its proper inclusion may play a role in the long time complete mixing observed in some of the experiments. While these issues are shared among many numerical problems, an additional complexity arising here concerns the initialization of the vortex ring when comparing to experimental data. Fortunately, given the time and length scales of this particular experiment (typically, in the order of seconds), direct numerical simulations do appear capable of resolving the fine structure in the evolution of vortex rings in stratified fluids (albeit, taking on the order of days for a single parallel simulation on a cluster).

In our case, an appropriate and convenient choice of a solver suitable for the numerical issues sketched above is offered by the VARDEN numerical code [6]. For the initialization of the numerical simulations, we use the Hill’s spherical vortex solution while tuning its free parameters to match the experimentally observed radius and velocity at a given position. Preliminary qualitative comparisons with the lab experiments have proven this toolset suitable to our purpose (see figure 9.2).

In this paper, we begin by introducing the problem and the governing equations. The numerical methods used to conduct direct numerical simulations of the full three-dimensional variable density Navier-Stokes equations are described in detail. These simulations will then be used to reproduce the critical phenomena of trap and escape which are observed in the experiments. We first first focus on the preliminary case of a
dense vortex ring in homogeneous ambient fluid and then probe the rich physical scenario ensuing from the interaction of the vortex ring and the ambient density transition layer.

9.2 Brief description of lab experiments

This section is a description of the experiments performed at the UNC Fluid lab by the experimental group. Experiments are carried out in a tank either filled with homogeneous or with two constant density layers separated by a sharp density transition. The setup is depicted in figure 9.3. The experiments consists in releasing drops of varying density from a prescribed height (typically 26 mm) above the free surface. In this way, after the drop splashes through the free surface, a coherent dense vortex ring forms in a quite repeatable manner after undergoing shedding process near the free surface (see figure 9.1).

The release height is selected to maximize the penetration depth and minimize at the same time the eccentricity of the droplet on impact, due to shape oscillations arising

![Figure 9.2: Example of a chandelier-like structure generated by the breaking of a vortex ring after impact on a sharp stratification. (a) Experimental, the green dye shows the high density fluid. (b) Density isosurfaces from 3D simulations, in a three-frames time sequence. Green corresponds to the high-density fluid threshold ($\rho \approx 1.03$) of the ring core, grey to an intermediate value in the transition layer ($\rho \approx 1.019$).](image)
Figure 9.3: Schematic of the experimental set up showing the tank, the IV line, and the syringe with linear drive.

<table>
<thead>
<tr>
<th>density [g/cc]</th>
<th>weight [g]</th>
<th>std dev.</th>
<th>average radius [cm]</th>
<th>std dev.</th>
</tr>
</thead>
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<td>0.00069</td>
<td>0.16079</td>
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<tr>
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<td>0.08374</td>
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</tr>
<tr>
<td>1.03979</td>
<td>0.07928</td>
<td>0.00064</td>
<td>0.15384</td>
<td>0.00038</td>
</tr>
</tbody>
</table>

Table 9.1: Droplet weight and radius measurements.

from surface tension for a droplet falling in air [27]. It turns out through empirical observations that the ideal configuration for the most coherent vortex ring occurs when the droplet impacts the surface transitioning from spherical to prolate spheroidal shape. This procedure leads to impact velocities on the order of $10^{-15}$ cm/sec, so that the Reynolds number based on droplet radius and impact velocity is $\approx 300 - 450$. The droplet release is controlled using a medical IV line connected to a small pipet. The IV line was then connected to a syringe attached to a precision manual linear drive which allowed for regular droplet creation. Droplet sizes are summarized in the table 9.1, created over an average of 35 drops.
The outlined experiment contains several dimensional parameters: $\rho_{\text{drop}}$, $\rho_T$, $\rho_B$, $R_{\text{drop}}$, $H_{\text{rel}}$, $H_t$, $H_b$, $\Delta$, where $\rho_{\text{drop}}$ is the droplet density, $\rho_T$ is the top layer density, $\rho_B$ is the bottom layer density, $R_{\text{drop}}$ is the droplet radius, $H_{\text{rel}}$ is the drop release height above the free surface, $H_t$ is the top layer thickness, $H_b$ is the bottom layer thickness, and $\Delta$ is the density transition length scale. In the case of a homogeneous ambient fluid, $\rho_T = \rho_B$ and $\Delta = 0$. For the purpose of this work we hold all parameters fixed except for $\rho_{\text{drop}}$ and $H_t$.

There exists a maximum penetration depth for a dense miscible vortex ring descending through a homogeneous fluid before the ring becomes unstable and breaks apart [27, 10]. The experiments quantify such maximum penetration length-scale in homogeneous ambient fluid. In contrast with vortex rings in homogenous fluids, the instability is here triggered by a Rayleigh–Taylor mechanism which sets in once the vortex motion is depleted by viscosity. This length scale sets the upper bound for top layer thicknesses which can be considered in the ambient sharply stratified case. Hence, in this set of experiments $\rho_T = \rho_B$ and $\rho_{\text{drop}}$ are varied. These simpler experiments are also used to compare to the direct numerical simulations making sure the code can accurately predict velocity and position of the vortex ring.

More details will be available in upcoming publications [19].

9.2.1 Critical phenomena: entrapment versus escape

The most important feature identified in the experiments with sharp internal stratification consists in the occurrence of two limiting behaviors, entrapment and escape, ensuing from the interaction of the vortex ring with the density transition layer. Figure 9.1 shows both behaviors in some detail. The first event is characterized by a complete entrapment of the high-density fluid (the green fluid in figure 9.1) above the background density transition layer. The typical dynamic preceding entrapment con-
sists of a partial entrainment of the “bubble”—i.e., the whole compound made of the vortex ring and the amount of upper-layer fluid dragged along by the ring—inside the bottom layer, followed by an upward bounce due to the overall positive buoyancy of the bubble. The second event, escape, is characterized by a complete entrainment of the vortex ring (and its bubble) below the transition layer; the factors that determine escape are probably high kinetic energetic of the vortex ring, and low potential energy penalty due to a smaller size of the bubble. (Notice in figure 9.1 the smaller ring size in the first frame of the bottom line compared to the first on top.) After a fairly deep penetration, the ring eventually becomes unstable and breaks apart, releasing the unmixed entrained light fluid in a rising plume. The high-density fluid resides permanently in the bottom layer.

In figure 9.4 it is reported a phase diagram showing the regions of trapping and escape in the \((\rho_{\text{drop}}, H_t)\) parameter space. Such diagram is based on a large number of experiments conducted in the UNC Fluid Lab.

### 9.3 Governing Equations

The governing equations for a stratified, incompressible fluid with variable density, are the following Navier-Stokes equations

\[
\begin{align*}
(\rho u)_t + (u \cdot \nabla) (\rho u) &= -\nabla p - g \rho \hat{z} + \mu \nabla^2 u, \\
\rho_t + u \cdot \nabla \rho &= 0, \\
\nabla \cdot u &= 0,
\end{align*}
\]  

(9.1)

where \(u\), \(\rho\), and \(\mu\) are the fluid velocity, density, and dynamic viscosity, respectively. The underlying assumption are that the dynamics take place on a scale fast enough to neglect diffusivity of the stratifying agents. Our fluids, being stratified with salt, do
Figure 9.4: Vortex ring critical length for trapping found from experiments, also shown in blue is the length of travel at which a vortex ring becomes unstable in a homogenous fluid, as well as $2/3$ scaling law prediction fit, which ignores the outlier which has critical length that falls within the density transition thickness. Also shown (red symbols) are the locations in the phase diagram of the companion numerical simulations. Notice that the distance, $L$, in the experimental data shown is measured from the free surface, whereas a fully formed vortex ring does not emerge until several radii below the free surface. (Experiments by R. Camassa, S. Khatri, R. McLaughlin, K. Mertens, D. Nenon and C. Smith.)

not involve any surface tension effects. We consider a three dimensional computational domain with periodic lateral boundary conditions on a square in the horizontal direction for both the velocity and density fields. The fluid domain is sandwiched between no-slip horizontal plates for the velocity field, and no-flux for the density field. Such boundary conditions only approximately represent the true physical boundary conditions, which in a fixed container should be no-slip for velocity and no-flux for density on all fixed walls. With a sufficiently large computational domain, however, the assumptions of periodicity often are a good approximation to the experimental setup. The initial conditions are chosen to emulate those of the experiment which involve an initial vortex whose core density is higher than all ambient fluid densities, with a given radius and velocity (described below in more detail). We remark that the initialization of the
vortex velocity and density field to reflect that of the experiment is a subtle issue, mainly due to experimental uncertainties.

The ambient fluid is either homogeneous, or a stably stratified density transition layer. A schematic of the two situations in which we present experimental and numerical results are shown in figure 9.5. The first case (left panel), in which a dense vortex ring settles in an ambient homogenous fluid, is used as a quantified, benchmark comparison between the experiment and the numerical simulation. Subsequently, the more complicated phenomenon emerging from a sharp background stratification (right panel) will be presented and compared to the data from a refined experimental campaign. These latter numerical studies, while preliminary, predict a striking critical phenomenon observed in the experiments. While in the experiment the density transition between the top and bottom ambient fluid layers has finite thickness, the numerical simulations are carried with a step density transition.

Figure 9.5: Schematic of the two cases presented in this paper. On the left panel, the case where a vortex ring with density, $\rho_{\text{drop}}$ is settling in homogeneous ambient fluid with density $\rho < \rho_{\text{drop}}$. On the right panel, a vortex ring with density, $\rho_{\text{drop}}$, is settling into a sharply stratified ambient fluid. The top layer has density, $\rho_T$, and the bottom layer has density, $\rho_B$, with $\rho_{\text{drop}} > \rho_B > \rho_T$. Here, we show a transition layer of finite thickness between the two densities, as occurs in experiments, but the numerical modeling is performed with zero thickness.
9.4 Numerical Method

For numerical simulations we employ a modified version of the software VARDEN developed at Lawrence Berkeley Lab [6]. We chose to use VARDEN as it is a reliable state of the art numerical code implemented for three dimensional large scale parallel computations that can handle variable density incompressible flows. The numerical scheme implemented in VARDEN is an approximate projection method, which employs a multigrid iterative linear solver to enforce incompressibility up to a prescribed tolerance. The advection terms in the momentum and density equations are discretized using a conservative second order upwind scheme with robustness properties suitable for non-diffusive density advection and even applicable in the limit of inviscid flows. Temporal evolution uses an adaptive time step set by user defined tolerances. For stability, momentum diffusion is treated implicitly with a Crank–Nicholson scheme. Further details on the method can be found in [6]. The simulations we perform have approximately $10^8$ grid points and take about one day to run (in wall-clock time) on a local UNC cluster typically running on 256, 2.93 GHz Intel processors. In the rectangular geometry described above, we employ rectangular uniformly-spaced meshes. Each timestep generates output files of 2.5 Gb typical size, and postprocessing the ensuing large dataset is efficiently handled using the Data Tank software package [3].

9.4.1 Initial conditions

To initialize the numerical simulation, the ambient stratification consists of constant density fluids either for the full computational domain, or configured as a step function at a prescribed height in the computational domain to model a sharp stratification. To initiate a downward propagating vortex ring, the velocity field is initialized using Hill’s spherical vortex exact solution [57]. This is a steady solution for homogeneous and inviscid fluids obtained by matching a rotational flow inside a sphere of radius $R_v$ with
an outer potential flow, to enforce continuity of velocity and pressure. Inside the sphere, the initial density, $\rho_{\text{drop}}$, is set to a constant value higher than all ambient densities, and consequently, this initial data is not an exact solution of either the inviscid or viscous dynamics. In this work, we adopt the lab reference system, in which the vortex travels with a vertical initial velocity, $U_0$. In the ensuing evolution the vortex ring shall expand and entrain ambient fluid, according to the general features of vortex ring dynamics. This will be illustrated and discussed below.

In three dimensions, Hill’s solution is expressed in terms of a suitably defined axial-symmetric streamfunction. The solution is

$$\psi(h, z) = \begin{cases} 
\frac{3}{4} U_0 h^2 \left( 1 - \frac{r^2}{R_v^2} \right) + \frac{1}{2} h^2 U_0 & \text{for } r < R_v, \\
-\frac{1}{2} U_0 h^2 \left( 1 - \frac{R_v^3}{r^3} \right) + \frac{1}{2} h^2 U_0 & \text{for } r > R_v,
\end{cases}$$

where $h$ is the distance from the axis of symmetry, $r = \sqrt{h^2 + (z - z_d)^2}$ is the distance from the center of the droplet, and

$$-\frac{1}{h} \frac{\partial \psi}{\partial z} = u_h, \quad \frac{1}{h} \frac{\partial \psi}{\partial h} = w$$

where $u_h$ and $w$ are the radial and vertical velocity components respectively. In cartesian coordinates the corresponding velocity field is

$$u = \frac{3}{2} U_0 \left( (x - x_d) \frac{z - z_d}{R_v^2}, \ (y - y_d) \frac{z - z_d}{R_v^2}, \ 1 - \frac{r^2 + h^2}{R_v^2} + \frac{2}{3} \right)$$

for $r < R_v$, and

$$u = \frac{3}{2} U_0 \left( (x - x_d) \frac{R_v^3}{r^5} (z - z_d), \ (y - y_d) \frac{R_v^3}{r^5} (z - z_d), \ \frac{2 R_v^3}{3 r^3} - h^2 \frac{R_v^3}{r^5} \right)$$
Figure 9.6: Instantaneous streamlines in the laboratory frame of Hill’s three-dimensional spherical vortex on the $x$-$z$ coordinate plane.

for $r > R_v$, where $x_d, y_d, z_d$ represent the center of the sphere. In Figure 9.6, the streamlines of the three dimensional Hill’s spherical vortex ring solution in the $x$-$z$ plane can be seen.

In order to compare numerical runs to lab experiments we need to reproduce initial conditions for the radius, velocity, and density of the vortex ring, that match the properties of the experimental vortex rings after their formation process is completed. The procedure we follow to obtain such initialization parameters is described in section 9.4.2.

9.4.2 The initial condition problem for the simulations

Quantitative comparison of a numerical simulation with a specific experiment, as mentioned above, requires an appropriate initial condition for the velocity, $U_0$, radius, $R_v$, and density of the Hill’s spherical vortex ring, $\rho_{\text{drop}}$. This information is not directly available from the current experimental setup due to the complex vortex formation processes associate with impacting the free surface. Imaging analysis provides partial information of these parameters, but is imprecise on account ambient fluid entrainment, optical aberrations, and dye dispersion. For the density, we choose to set the Hill’s
spherical vortex ring density, \( \rho_{\text{drop}} \), to be identical to the initial experimental drop density. Often experiments with identical conditions were replicated numerous times. In these cases, the average value of the measured radii and velocities were used to set the initial conditions of the simulation with identical parameters.

The position of the vortex ring and the resulting behaviors as it evolves in time are highly dependent on the initialization of the vortex ring. In the numerical simulations, we are using the inviscid steady state solution, the Hill’s spherical vortex ring, to initialize the problem. By using this initial condition, we are assuming that the vortex ring is quickly evolving into a solution of the viscous variable density Navier–Stokes equations. Thus, we set the radius and velocity in the initial Hill’s vortex ring in the simulations based on the fully formed vortex ring observed in the experiments. Ideally, it would be desirable to set the initial conditions of the numerical simulations on a fully developed viscous solution emanating from the Hill spherical vortex. Lacking full experimental information regarding the evolving velocity and density field, and establishing a numerical procedure for carrying out a precise initial condition matching, we defer this improvement to future studies.

### 9.5 Simulations

The primary goal of numerical simulation is to demonstrate the phenomenology observed in experiments. We stress once more how the numerical setup is an approximation of the actual experimental conditions. Nonetheless, we are able to reproduce comparable behaviors and trends with respect to parameter changes.

The numerical results are organized in two sections. The first contains preliminary simulations in a homogeneous environment, which mostly serve as reference. The second contains the simulations of the sharply-stratified tank experiments.
9.5.1 Vortex ring dynamics: homogeneous environment

To verify the numerical simulations conducted using the methodology presented in Section 9.4, we first compare simulations and experiments of vortex rings descending in a homogeneous ambient fluid. To compare a simulation with a set of experiments, the ambient fluid density is set as in the experiments, and the vortex density is set as described above in section 9.4.2. We choose values for the initial radius and velocity based on the imaged experimental vortex ring radius and velocity shortly after the drop has passed through the free surface and rolled into a vortex ring. During this process the drop sheds a minimal amount of fluid which can visually be seen.

Figure 9.7: Comparisons of simulations and experiments of varying density drops into freshwater. Top: 1.02 g/cc drop, Bottom: 1.04 g/cc drop. (Simulations by S. Khatri.)
In figure 9.7, the position and velocity of the descending vortex ring averaged over ten identical experiments and the position and velocity of the vortex ring in numerical simulations are shown. These simulations target two different density drops, $\rho_{\text{drop}}$, 1.02 g/cc and 1.04 g/cc, being released in freshwater ambient fluid. Following the initialization procedure discussed above in §9.4.2, we set the initial radius of the Hill’s vortex ring to $R_v = 0.225$ cm and the initial downward velocity to $U_0 = 10.4$ cm/s for the case of a 1.02 g/cc drop. Similarly, for the case of a 1.04 g/cc drop, the initial radius is set to $R_v = 0.204$ cm and the initial velocity to $U_0 = 10.0$ cm/s. In these simulations, the grid is selected as in the benchmark above.

As can be seen, there is reasonable quantitative agreement between the simulation and experiments, which verifies the methodology of the simulations presented here. The numerical simulations accurately captures the behavior of the vortex ring as it descends. Notice that the initial velocity is slightly different in the simulation with respect to the experimental values. This discrepancy is most likely due to the difficulty of setting initial conditions, as described in section 9.4.2.

9.5.2 Vortex ring dynamics: stratified environment

In this section we present numerical computations including a sharp internal stratification in the simulated tank. We now set an upper layer density equal to 1.00 g/cc, as for the unstratified case, above a lower layer where $\rho = 1.02$ g/cc. We consider a droplet of density equal to 1.03 g/cc. This choice is motivated by the experiments. These demonstrate that there is a critical behavior which can be summarized in the phase diagram shown in figure 9.4: as the density contrast changes, the critical lengths vary.

In the following runs, the size of the computational domain is set to be $L_H \times L_H \times 5L_H$ with $L_H = 8R_v$, discretized on uniform meshes of size $n_x \times n_y \times n_z$ (see table 9.2). Two
Table 9.2: Dimensional parameters used in the numerical runs with internal stratification, units are cm, s, g.

<table>
<thead>
<tr>
<th>Run</th>
<th>$R_v$</th>
<th>$U_0$</th>
<th>$H_t$</th>
<th>$\rho_T$</th>
<th>$\rho_B$</th>
<th>$\rho_{\text{drop}}$</th>
<th>Grid size ($n_x$)</th>
<th>Interface</th>
<th>Behavior</th>
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<tr>
<td>1</td>
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<td>25</td>
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<td>1</td>
<td>1.02</td>
<td>1.03</td>
<td>256</td>
<td>Sharp</td>
<td>Escape</td>
</tr>
<tr>
<td>2</td>
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<td>25</td>
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<td>1</td>
<td>1.02</td>
<td>1.03</td>
<td>256</td>
<td>Sharp</td>
<td>Bounce</td>
</tr>
<tr>
<td>3</td>
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<td>25</td>
<td>3.6</td>
<td>1</td>
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<td>1.03</td>
<td>256</td>
<td>Smooth</td>
<td>Bounce</td>
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<tr>
<td>4</td>
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<td>1</td>
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<td>1.03</td>
<td>512</td>
<td>Smooth</td>
<td>Bounce</td>
</tr>
</tbody>
</table>

cases will be studied, the first which depicts an escaping vortex ring, and the second demonstrates a trapping.

Physical parameters are reported in table 9.2. Notice that the Hill’s spherical vortex is always initialized with its center located at a $4R_v$ distance below the top of the computational domain, so that $H_t - 4R_v$ is the distance from the vortex center to the transition layer at $t = 0$.

In figure 9.8 the outcome of the first simulation (run 1) is depicted as a time series plotting level sets of intermediate density values (grey marking near top layer density values of 1.018g/cc, and green marking near core density values of 1.025 g/cc). This case documents the complete escape of a vortex ring through the density transition. In contrast, Figure 9.9, depicts the second case (run 2) demonstrating trapping: as the vortex passes through the density transition, the entrainment bubble of light upper fluid carries all of the dense core back up into the density transition region.

The numerical flow visualizations allow to observe clearly the process of entrainment of a bubble of top layer light fluid below the transition layer, which is a crucial aspect of the process. Figure 9.8 allows to appreciate the kinematic of the entrainment process, which proceeds by “wrapping” around the vortex ring new shells of surrounding fluid. The bubble visualized by the grey level-set in the snapshot at $t = 0.1651$ contains
upper-layer fluid previously entrained in the bubble during its propagation through the upper layer. The snapshot at \( t = 0.2675 \) shows how such process continues even after the vortex ring penetrates inside the bottom layer, in particular the cross section of the grey level-set makes evident a spiraling structure—footprint of entrainment. The ongoing entrainment of bottom-layer fluid builds up a new outer-shell around the grey level-set, which assumes a toroidal shape (see the snapshots at and \( t = 0.6123 \)). Eventually, the energy of the vortex ring is dissipated by viscosity. When this happens (see snapshot at \( t = 1.153 \)) the positive buoyancy of low-density fluid contained in the bubble prevails in the balance of forces, and an ascending buoyant plume is released (last snapshot).

For run 2, in contrast, the bubble entrainment generates the buoyancy-driven rebound. In this case the strong rebound destroys the ring structure, and drags back up the high-density fluid contained inside the ring core.

The effect of layer thickness in the ambient stratification has been explored in run 3, see figure 9.10. For the smooth density profile

\[
\rho(y) = \rho_T + \frac{1}{2}(\rho_B - \rho_T) \left[ 1 - \tanh \left( \frac{z - z_t}{2} \right) \right]
\]

has been used in such runs, where \( z_t \) is the vertical position of the transition layer located at a \( H_t \) distance from the top of the domain. This finite thickness of the transition layer seems to play a secondary role. The details of the structure of the trapped high-density fluid appears to be the most visible difference between runs 2 and 3.

### 9.5.3 Some comments about resolution effects

The \( n_x = 256 \) grid has been assumed to yield an acceptable working resolution throughout the above numerical study of vortex ring dynamics. The assumption was
based on a few comparisons with runs using lower resolution, which didn’t show
dramatic changes in the main physical features. In this section we present some further
numerical tests aimed to better assess the validity of such assumption. The run giving
rise to a bounce event (run 3) has been replicated with doubled spatial resolution (run
4), keeping all physical parameters unchanged. To reduce the very high computational
cost of such run, we have exploited the symmetry of the problem about the $x - z$ and
$y - z$ planes intersecting the center line, and we have resolved only one quarter of the
domain enforcing symmetry through the boundary conditions.

A comparison between the high-resolution ($n_x = n_y = 512$) and the regular-
resolution ($n_x = n_y = 256$) simulations is offered in figure 9.11. Overall, the change of
resolution is seen to preserve the main physical features. In particular, the two runs
are virtually identical until $t \approx 1$, i.e., until the bouncing process gives rise to a strong
stretching of the fluid elements. At later times stronger differences appear on several
details. For instance, it is clearly observable that numerical diffusion has produced
more smoothing of the high-density filaments in run 3 (see the $t \approx 1.2$ snapshots in
figure 9.11). The ultimate consequence of having less artificial diffusion appears to be
a larger amount of unmixed heavy fluid, which eventually sinks in the bottom layer
for long times. This result, which brings on surface a fundamental difference between
simulations and experiments, should not be immediately interpreted as a pitfall of this
study. In fact, it may be a hint for a better understanding of the relation between the
lab experiments and the model set-up devised for the simulations. This point will be
better explained in the conclusive discussion in §9.6.

9.6 Discussion

A series of direct numerical simulations of dense-core vortex rings descending through
a sharply stratified density transition has been performed. Overall we achieved an excel-
lent qualitative agreement with experiments. In particular, the critical escape/trapping phenomena summarized in the experimental phase diagram are confirmed. From the quantitative point of view we obtained, at least, a good correlation between the different regimes and the corresponding settings of physical parameters.

Both events are characterized by stirring and filamentation of the dense fluid to scales on which molecular diffusion wipes out buoyancy differences. It is likely that numerical diffusivity becomes consistent in the later stage, as very small structures are created. This is also hinted by visualizations (figures 9.8 and 9.9) clearly showing smaller volumes of high-density fluid in the latest frames.

In all simulations presented, finite-domain effects do not seem to play a significant role in the dynamics, even though a systematic verification remains to be done. One fact suggesting that boundary effects are negligible is that the axial symmetry of the initial condition is broken by the geometry of the computational domain, yet the vortex ring remains essentially axial symmetric until destabilization occurs. The structure ensuing from the vortex break-up maintains a four-fold symmetry imposed by the domain shape. Bottom effects have been observed at longer time. In figure 9.8 the domain bottom lies close below the density “fingers” shown in the last frame (about a $R_v$ distance). The impact of the high-density drops on the bottom is visible at later times (not shown here).

One of the major discrepancies between simulations and experiments lie in the overall amount of mixing: experiments exhibit more mixing than simulations. In the experiments showing bounce phenomena, the trapped fluid remains above (or within) the transition layer (in the experiments such layer has always a finite thickness) for an indefinite amount of time. In other words, trapping appears to be permanent. This was never the case in the simulations performed by far, where some part of the high-density fluid remains unmixed and eventually sinks through the bottom layer on longer
time scales. The reasons of this fact are not completely clear, but it is reasonable to expect experiments to contain additional sources of noise, resulting in more mixing. In particular, mixing can be expected to occur during the initial roll-up of vortex rings right after the impact of the droplet on the free surface, so that the assumption of an unmixed plug of high-density fluid in the numerical initial condition could introduce a significant bias. This issue should be better investigated in future work.

These results demonstrate large scale computing’s capability for producing quantified predictions of some complex stratified fluid behavior. This investigation sheds light on the applicability of direct numerical simulations to physical problems of great importance, such as mixing in stratified jets and plumes, central to numerous environmental and geophysical problems for the example of plume formation in oil spills).
Figure 9.8: Vortex escaping through the step-function internal stratification (run 1), visualized by density isosurfaces. Green $\rho = 1.025$; grey $\rho = 1.018$. 
Figure 9.9: Vortex trapping through the step-function internal stratification (run 2), visualized by density isosurfaces. Green $\rho = 1.025$; grey $\rho = 1.018$. 
Figure 9.10: Vortex trapping through a smooth internal stratification (run 3), visualized by density isosurfaces. Green $\rho = 1.025$; grey $\rho = 1.018$. 
Figure 9.11: Vortex trapping through a smooth internal stratification. Comparison between $n_x = 256$ resolution (left column, run 3) and $n_x = 512$ resolution simulations (right column, run 4). Green $\rho = 1.025$; grey $\rho = 1.018$. 
Appendix A

SLOW-VARYING MEDIA ASYMPTOTICS FOR WEAKLY NON-PARALLEL STRATIFIED SHEAR FLOWS (APPENDIX TO PART I)

In this appendix it is reported a calculation leading to an envelope equation for linear perturbations in wave-induced shear flows, under the assumption of slow-varying background flow. The three-layer configuration defined in §3.1.1, in which the flow field is partitioned into three regions separated by the internal interfaces $\zeta_1$ and $\zeta_2$, will be understood in what follows.

A.1 Multiscale method in weakly non-parallel stratified flows

We first adopt the usual decomposition of all dependent variables into a base state and a perturbation

\[ u = U + u', \quad v = V + v', \quad p = P + p', \quad \rho = R + \rho', \quad \zeta_i = N_i + \eta_i. \]

According to the multiple-scale method we assume asymptotic expansions in the following form for all perturbative quantities

\[ u = u^{(0)}(x,y,t,X,T) + \epsilon u^{(1)}(x,y,t,X,T) + O(\epsilon^2). \]
The governing equations (1.2) are linearized about the base state and the above assumption are used. Any time a derivative with respect to \(x\) or \(t\) appears, it is transformed according to the rule

\[
\frac{\partial}{\partial x} \rightarrow \frac{\partial}{\partial x} + \epsilon \frac{\partial}{\partial X}, \quad \frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial T}.
\]

By collecting all terms multiplied by identical powers of \(\epsilon\), we find at \(O(1)\)

\[
\eta_i^{(0)} + U\eta_i^{(0)} = v^{(0)}, \quad (A.3)
\]

\[
u_t^{(0)} + U\nu_x^{(0)} + v^{(0)}U_y = -\frac{1}{\rho_0}p_x^{(0)}, \quad (A.4)
\]

\[v_t^{(0)} + Uv_x^{(0)} = -\frac{1}{\rho_0}p_y^{(0)} - \frac{a}{\rho_0}\rho^{(0)}. \quad (A.5)
\]

At \(O(\epsilon)\) only the equation for the horizontal momentum will be needed (the reason shall be apparent from the developments of the calculations), which turns out to be

\[
u_t^{(1)} + u_t^{(0)} + Uu_x^{(1)} + Uu_x^{(0)} + v^{(1)}U_y + Vu_y^{(0)} + U_X u^{(0)} = -\frac{1}{\rho_0} (p_X^{(0)} + p_x^{(1)}) \quad (A.6)
\]

The conditions to be imposed at the interfaces at any order are obtained from expanding (3.4). The internal interfaces \(\eta_i\) are assimilated to the unperturbed interfaces \(N_i\) as the theory is leading-order in the amplitude of the perturbations. Observing that the unit vectors normal and tangent to \(N_i\) are

\[
n = -\epsilon N_x x + y \sqrt{\epsilon^2 N^2_x + 1}, \quad \tau = x + \epsilon N_y y \sqrt{\epsilon^2 N^2_x + 1}.
\]
the expansion of (3.4) can be easily obtained. At $O(1)$ one finds

$$
(u \cdot n)^{(0)} = v^{(0)},
$$

(A.7)

$$
(\nabla p \cdot \tau)^{(0)} = p_x^{(0)},
$$

(A.8)

and at $O(\epsilon)$

$$
(u \cdot n)^{(1)} = -u^{(0)} N_X^{(0)} + v^{(1)},
$$

(A.9)

$$
(\nabla p \cdot \tau)^{(1)} = p_x^{(1)} + p_X^{(0)} + p_y^{(0)} N_X.
$$

(A.10)

The above quantities are enforced to be continuous across $N_i$.

For the rest of the analysis we will work with the streamfunction representation. The first two orders in the $\epsilon$-expansion of $\psi$ are related to velocity by

$$
\psi_y^{(0)} = u^{(0)}, \quad \psi_x^{(0)} = -v^{(0)}
$$

(A.11)

$$
\psi_y^{(1)} = u^{(1)}, \quad \psi_x^{(1)} + \psi_X^{(0)} = -v^{(1)}
$$

(A.12)

In order to proceed in the analysis we particularize the perturbations ansatz (A.2) to that of slowly modulated wave packets (see, e.g., [76])

$$
\psi = \left( \hat{\psi}^{(0)} + \epsilon \hat{\psi}^{(1)} \right) e^{\theta(x,t)} + O(\epsilon^2),
$$

(A.13)

$$
\rho = \left( \hat{\rho}^{(0)} + \epsilon \hat{\rho}^{(1)} \right) e^{\theta(x,t)} + O(\epsilon^2),
$$

(A.14)

where $\hat{\psi}^{(n)} = \hat{\psi}^{(n)}(y, X, T)$ (and similarly for $\hat{\rho}^{(n)}$) and the complex phase-function $\theta$ is associated to the concept of local wavenumber and frequency in the usual way

$$
\theta_x = i k(X, T), \quad \theta_t = -i \omega(X, T).
$$
The construction is completed by the consistency relation

\[ k_T = -\omega_X \]  \hspace{1cm} (A.15)

that guarantees \( \theta \) to be a well-defined function of \( x \) and \( t \).

After further manipulations are carried through (reported separately in the next section §A.2), one obtains a hierarchy of boundary value problems with mixed (Robin) boundary conditions. At \( O(1) \) we find the local parallel problem

\[ \mathcal{L} \hat{\psi}^{(0)}_M = 0, \quad \mathcal{U} \hat{\psi}^{(0)}_M = 0, \]  \hspace{1cm} (A.16)

and at \( O(\epsilon) \)

\[ \mathcal{L} \hat{\psi}^{(1)} = \text{RHS}, \quad \mathcal{U} \hat{\psi}^{(1)} = \text{NH}, \]  \hspace{1cm} (A.17)

where

\[ \text{RHS} = -(i\mathcal{L}_\omega \partial_T - i\mathcal{L}_k \partial_X - i\frac{1}{2} \mathcal{L}_{kk} k X + i\frac{1}{2} \mathcal{L}_{\omega\omega} \omega_T + i\frac{1}{2} \mathcal{L}_{\omega k} (k_T - \omega_X) + \mathcal{L}_\epsilon) \hat{\psi}^{(0)} \] \hspace{1cm} (A.18)

\[ \text{NH} = -(i\mathcal{U}_\omega \partial_T - i\mathcal{U}_k \partial_X - i\frac{1}{2} \mathcal{U}_{kk} k X + i\frac{1}{2} \mathcal{U}_{\omega\omega} \omega_T + i\frac{1}{2} \mathcal{U}_{\omega k} (k_T - \omega_X) + \mathcal{L}_\epsilon) \hat{\psi}^{(0)} \] \hspace{1cm} (A.19)

In the above formulas, boundary conditions are expressed in a somewhat abstract notation using boundary forms. This allows to write the final products of this analysis in a more compact way. Boundary forms \( (\mathcal{U}, \mathcal{U}_\omega, \mathcal{U}_k, ...) \) are thought of as linear operators acting on the \( \hat{\psi} \)'s functions, which return the necessary linear combinations of such functions and their derivatives evaluated at the boundaries to express boundary conditions. The boundary forms are specified by the matrix representations:
\[ \mathbf{U}_\psi \equiv \begin{bmatrix} kU_{1y} - k^2U_1 + k\omega & 0 & -kU_1 + \omega & 0 \\ 0 & -kU_{2y} - k^2U_2 + k\omega & 0 & kU_2 - \omega \end{bmatrix} [\psi],\]

\[ \mathbf{U}_k\psi \equiv \begin{bmatrix} U_{1y} - 2kU_1 + \omega & 0 & -U_1 & 0 \\ 0 & -U_{2y} - 2kU_2 + \omega & 0 & U_2 \end{bmatrix} [\psi],\]

\[ \mathbf{U}_\omega\psi \equiv \begin{bmatrix} k & 0 & 1 & 0 \\ 0 & k & 0 & -1 \end{bmatrix} [\psi],\]

\[ \mathbf{U}_{kk}\psi \equiv \begin{bmatrix} -2kU & 0 & 0 & 0 \\ 0 & -2kU & 0 & 0 \end{bmatrix} [\psi],\]

\[ \mathbf{U}_{k\omega}\psi \equiv \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} [\psi],\]

\[ \mathbf{U}_\varepsilon\psi \equiv i \begin{bmatrix} k(U_{1x} + N_{1x}U_y) & 0 \\ 0 & k(U_{2x} + N_{2x}U_y) \end{bmatrix} \]

\[ \mathbf{U}_{1x} + N_{1x}(kU_1 - U_y) & 0 & N_{1x}U_1 & 0 \\ 0 & -U_{2x} + N_{2x}(kU_2 + U_y) & 0 & -N_{2x}U_2 \end{bmatrix} [\tilde{\psi}],\]

where \([\psi] = [\psi_1 \psi_2 \psi_{1y} \psi_{2y}]^T\) and \([\tilde{\psi}] = [\psi_1 \psi_2 \psi_{1y} \psi_{2y} \psi_{1yy} \psi_{2yy}]^T\).

The \(O(\varepsilon)\) non homogeneous problem requires a solvability condition to be satisfied by the right-hand side of both the differential and the boundary form parts. Such condition is given as \((\text{Coddington }&\text{ Levinson [30]})\)

\[ (\text{RHS}, \hat{\psi}^\dagger) - NH \cdot \mathbf{U}_\varepsilon^\dagger \hat{\psi}^\dagger = 0, \quad (A.20) \]
where $\mathcal{U}_c^\dagger$ is the boundary form complementary-adjoint to $\mathcal{U}$, and $\hat{\psi}^\dagger$ is an eigenfunction of the adjoint boundary value problem defined by $\mathcal{L}^\dagger$ and $\mathcal{U}^\dagger$. Definitions and method to determine $\mathcal{U}_c^\dagger \hat{\psi}^\dagger$ are reported in §A.3.2.

Condition (A.20) yields an expression that involves integral operators on $\hat{\psi}_M^{(0)}$ (essentially the same that appears in analogous but unbounded problems, see, e.g., Saric & Nayfeh [82] ), plus a discrete part that derives from the boundary conditions term and contains the values of $\hat{\psi}_M^{(0)}$ and its derivatives in $y$ at the boundaries. In a single-mode perturbation the vertical $y$-structure, which is determined by the $O(1)$ eigenvalue problem, cannot change in time. Hence the streamfunction is further separated as

$$
\hat{\psi}^{(n)} = A_n \phi_n, \quad \hat{\rho}^{(n)} = B_n \chi_n,
$$

where $A_n = A_n(X,T), \phi_n = \phi_n(y,X,T)$ (and similarly for $B_n$, and $\chi_n$) After some laborious though straightforward manipulations are carried through, and using the expression (A.46) for the group velocity $\Omega_k$, the solvability condition (A.20) yields an evolutive equation for the envelope function:

$$
A_T + \Omega_k A_X + (\gamma_1 + \gamma_2)A + \sigma_1 k_T A + \sigma_2 k_X A = 0.
$$

The coefficients $\gamma_1$, $\gamma_2$ and $\sigma$ in the above equation are given as

$$
\begin{align*}
\gamma_1 &= \left[ (\mathcal{L}_\omega \phi_T, \phi_T^\dagger) - (\mathcal{L}_k \phi_X, \phi_X^\dagger) - \mathcal{U}_\omega \phi_T \cdot \mathcal{U}_c^\dagger \phi_T^\dagger + \mathcal{U}_k \phi_X \cdot \mathcal{U}_c^\dagger \phi_X^\dagger \right] \left[ (\mathcal{L}_\omega \phi, \phi^\dagger) - \mathcal{U}_\omega \phi \cdot \mathcal{U}_c^\dagger \phi^\dagger \right]^{-1} \\
\gamma_2 &= -i \left[ (\mathcal{L}_\epsilon \phi, \phi^\dagger) - \mathcal{U}_\epsilon \phi \cdot \mathcal{U}_c^\dagger \phi^\dagger \right] \left[ (\mathcal{L}_\omega \phi, \phi^\dagger) - \mathcal{U}_\omega \phi \cdot \mathcal{U}_c^\dagger \phi^\dagger \right]^{-1} \\
\sigma_1 &= -i \left[ (\mathcal{M}_t \phi, \phi^\dagger) \right] \left[ (\mathcal{L}_\omega \phi, \phi^\dagger) - \mathcal{U}_\omega \phi \cdot \mathcal{U}_c^\dagger \phi^\dagger \right]^{-1} \\
\sigma_2 &= -i \left[ (\mathcal{M}_x \phi, \phi^\dagger) - \mathcal{V} \phi \cdot \mathcal{U}^\dagger \right] \left[ (\mathcal{L}_\omega \phi, \phi^\dagger) - \mathcal{U}_\omega \phi \cdot \mathcal{U}_c^\dagger \phi^\dagger \right]^{-1}
\end{align*}
$$

(A.21) (A.22) (A.23) (A.24)
A.2 Details of the derivation

A.2.1 Continuous part: stability operators

In two dimensions the Boussinesq equation of motion in the vorticity formulation read

\[ \partial_t \nabla^2 \psi + J(\psi, \nabla^2 \psi) = g \partial_x \rho \]  \hspace{1cm} (A.25)
\[ \partial_t \rho + J(\psi, \rho) = 0 \]  \hspace{1cm} (A.26)

where the Jacobian \( J \) used to express the convective terms is defined as the bilinear form \( J(f, g) = f_y g_x - f_x g_y \). We introduce the decomposition into a background steady-state flow and a perturbation

\[ \psi = \Psi + \psi', \quad \rho = R + \rho', \]

where the primed variables represent the perturbation. Since we will not be concerned with the total variables (\( \psi \) and \( \rho \)) any more, we immediately drop the primes (‘) for the perturbative variables. The equations governing the evolution of the perturbation are easily obtained and read

\[ \partial_t \nabla^2 \psi + J(\Psi, \nabla^2 \psi) + J(\psi, \nabla^2 \psi) + J(\psi, \nabla^2 \psi) = g \partial_x \rho, \] \hspace{1cm} (A.27)
\[ \partial_t \rho + J(\Psi, \rho) + J(\psi, R) + J(\psi, \rho) = 0. \] \hspace{1cm} (A.28)

(The primes, again, will be dropped from now on.) After the non-dimensionalization and the transformations of derivatives are performed, the resulting equations are conveniently written, following Huerre \textit{et al.} [76], splitting all differential operators as to separating the orders of magnitude in \( \epsilon \). Retaining only terms up to first order we
\[
\begin{align*}
\partial_t & \quad -i\omega & \quad \partial_T \\
\partial_x & \quad ik & \quad \partial_X \\
\partial_t \nabla^2 & \quad i\omega(k^2 - \partial_{yy}) & \quad \omega(2k\partial_X + k_X) + (k^2 - \partial_{yy})\partial_T - 2kk_T \\
\mathcal{D}_{11} & \quad [\Psi_y(-k^2 + \partial_{yy}) - \Psi_{yyy}]ik & \quad \Psi_y(-3k^2\partial_X - 3kk_X + \partial_{yy}\partial_X) - \Psi_{yyy}\partial_X \\
\mathcal{D}_{11e} & \quad -\Psi_X\partial_y(-k^2 + \partial_{yy}) + \Psi_{yyX}\partial_y & \quad -\Psi_X\partial_y ik\partial_X \\
\mathcal{D}_{12} & \quad -gik & \quad -g\partial_X \\
\mathcal{D}_{22} & \quad \Psi_y ik & \quad \Psi_y\partial_X \\
\mathcal{D}_{22e} & \quad -\Psi_X\partial_y & \quad - \\
\mathcal{D}_{21} & \quad -R_y ik & \quad -R_y \partial_X \\
\mathcal{D}_{21e} & \quad R_X\partial_y & \quad - \\
\end{align*}
\]

Table A.1: First two terms in the $\epsilon$-expansions for all operators.

\[
\begin{align*}
\partial_t \nabla^2 \psi + \mathcal{D}_{11} \psi + \epsilon \mathcal{D}_{11e} \psi + \mathcal{D}_{12} \rho + O(\psi^2) + O(\epsilon^2) & = 0 \\
\partial_t \rho + \mathcal{D}_{22} \rho + \mathcal{D}_{21} \psi + \epsilon \mathcal{D}_{22e} \rho + \epsilon \mathcal{D}_{21e} \psi + O(\psi \rho) + O(\epsilon^2) & = 0
\end{align*}
\]

where all the operators are

\[
\begin{align*}
\mathcal{D}_{11} & = \Psi_y \partial_x \nabla^2 - \Psi_{yyy} \partial_x, & \mathcal{D}_{11e} & = -\Psi_X \partial_y \nabla^2 + \Psi_{yyX} \partial_y, \\
\mathcal{D}_{12} & = -g\partial_x, & \mathcal{D}_{22} & = \Psi_y \partial_x, & \mathcal{D}_{22e} & = -\Psi_X \partial_y \\
\mathcal{D}_{21} & = -R_y \partial_x, & \mathcal{D}_{21e} & = R_X \partial_y.
\end{align*}
\]

Those labeled by epsilon ($\epsilon$) contain the $O(\epsilon)$ non-parallel effects.

The functions $\phi$'s and $\chi$'s are normalized to have unitary $L_2$ norm. Notice that $\theta$ depends on the fast coordinates, meaning that its first derivatives are $O(1)$ in $\epsilon$, but each further derivation lowers the order of magnitude by a factor $\epsilon$. After the solution is restricted to the above form we can carry further the splitting into different orders in $\epsilon$ of all the $\mathcal{D}$’s operator. These are summarized in Table A.1.
All linear operators involved in this procedure can be expanded in $\epsilon$ as

$$\mathcal{L} = \mathcal{L}^0[k, \omega] + \epsilon\mathcal{L}^1[k, \omega] + \ldots,$$

and it can be observed that, assuming the ansatz (A.13) and (A.14), the following rule holds

$$\mathcal{L}^1 = -i\mathcal{L}_k^0 \partial_X + i\mathcal{L}_\omega^0 \partial_T - i\frac{1}{2}\mathcal{L}_{kk}^0 k X + i\frac{1}{2}\mathcal{L}_{\omega\omega}^0 \omega T + i\frac{1}{2}\mathcal{L}_{kk}^0 (k T - \omega X).$$

(A.29)

Notice that we did not use the obvious substitution $(k T - \omega X) = 2k T$ in order to emphasize the underlying pattern. Using the above observation we can derive, for later reference, the following identity which holds for the pairing $(\mathcal{L}^1 \psi, \phi^\dagger)$ when $\psi$ has the structure $\psi = A(X, T) \phi(y, X)$, and when $\phi$ ($\phi^\dagger$) is an eigenfunction of $\mathcal{L}^0$ ($\mathcal{L}^0$)

$$\langle \mathcal{L}^1 \psi, \phi^\dagger \rangle = - (i\mathcal{L}_k^0 \phi, \phi^\dagger) A_X - (i\mathcal{L}_\omega^0 \phi_X, \phi^\dagger) A
\]

$$+ (i\mathcal{L}_\omega^0 \phi_T, \phi^\dagger) A
\]

$$- i\frac{1}{2} (L_{kk}^0 \phi, \phi) A + i\frac{1}{2} (L_{\omega\omega}^0 \omega T \phi, \phi) A + i\frac{1}{2} (L_{kk}^0 (k T - \omega X) \phi, \phi) A$$

(A.30)

where (A.46) has been used and

$$\gamma_1 = \frac{\langle L_{\omega}^0 \phi_X, \phi^\dagger \rangle - \langle L_{k}^0 \phi_X, \phi^\dagger \rangle}{\langle L_{\omega}^0 \phi, \phi^\dagger \rangle}. \quad \text{(A.31)}$$

Using the expansions (A.13)-(A.14) into the governing equations a hierarchy of problems is obtained. At $O(1)$ one finds the local parallel problem:

$$\left( \partial_t \nabla^2 \right)^0 \hat{\psi}^{(0)} + D_{11}^0 \hat{\psi}^{(0)} + D_{12}^0 \hat{\rho}^{(0)} = 0$$

$$- ikc \hat{\rho}^{(0)} + D_{22}^0 \hat{\rho}^{(0)} + D_{21}^0 \hat{\psi}^{(0)} = 0$$

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solving the second equation for the density

\[ \hat{\rho}^{(0)} = - \frac{D_{21}}{D_{22} - i\omega} \hat{\psi}^{(0)} = \frac{kR_y}{k\Psi_y - \omega} \hat{\psi}^{(0)} \]

we obtain the local parallel Taylor-Goldstein eigenvalue problem

\[ \mathcal{L}^{(0)} \hat{\psi}^{(0)} = 0 \]

where

\[ \mathcal{L}^{(0)} = (k\Psi_y - \omega)(-k^2 + \partial_{yy}) - k\Psi_{yyy} - \frac{k^2gR_y}{k\Psi_y - \omega}. \]

The solution of the \( O(1) \) problem yields the local dispersion relation \( \Omega(k, X) = \omega(X, T) \), that with (A.15) provides the well-known evolution equation for \( k \) in non-homogeneous media

\[ k_T + \Omega k_k + \Omega_X = 0. \]

At \( O(\epsilon) \) the linearized equations are

\[
\begin{align*}
(\partial_t \nabla^2)^0 \hat{\psi}^{(1)} + D_{11}^0 \hat{\psi}^{(1)} + D_{12}^0 \hat{\rho}^{(1)} &= -D_{11}^0 \hat{\psi}^{(0)} - (\partial_t \nabla^2)^1 \hat{\psi}^{(0)} - D_{11}^1 \hat{\psi}^{(0)} - D_{12}^1 \hat{\rho}^{(0)} \\
-i\omega \hat{\rho}^{(1)} + D_{22}^0 \hat{\rho}^{(1)} + D_{21}^0 \hat{\psi}^{(1)} &= -D_{21}^0 \hat{\psi}^{(0)} - D_{22}^0 \hat{\rho}^{(0)} - \partial_T \hat{\rho}^{(0)} - D_{22}^1 \hat{\rho}^{(0)} - D_{21}^1 \hat{\psi}^{(0)};
\end{align*}
\]

solving for \( \hat{\rho}^{(1)} \) the second one we obtain

\[ \hat{\rho}^{(1)} = \frac{D_{21}^0}{i\omega - D_{22}^0} \hat{\psi}^{(1)} + \frac{D_{21}^0 \hat{\psi}^{(0)} + D_{22}^0 \hat{\rho}^{(0)} + \partial_T \hat{\rho}^{(0)} + D_{22}^1 \hat{\rho}^{(0)} + D_{21}^1 \hat{\psi}^{(0)}}{i\omega - D_{22}^0}. \]

Use this result inside the first equation a non-homogeneous equation for \( \hat{\psi}^{(1)} \) is obtained

\[ \mathcal{L}^{(0)} \hat{\psi}^{(1)} = -(\mathcal{L}^{(1)} + \mathcal{L}_e) \hat{\psi}^{(0)} \]  

(A.32)
where the right-hand operators contain the slow terms and nonparallel corrections respectively:

\[
\mathcal{L}^{(1)} = (\partial_t \nabla^2)^{1} + D_{11}^{1} + \frac{D_{12}^{1} D_{21}^{0}}{i \omega - D_{22}^{0}} + \frac{D_{12}^{0} D_{21}^{1}}{i \omega - D_{22}^{0}} - \frac{D_{12}^{0} D_{21}^{0} (\partial_T + D_{22}^{1})}{(i \omega - D_{22}^{0})^2}
\]

\[
\mathcal{L}_\epsilon = D_{11}^{0} + \frac{D_{12}^{0} D_{21}^{0} \epsilon}{i \omega - D_{22}^{0}} - \frac{D_{12}^{0} D_{21}^{0} D_{22}^{0}}{(i \omega - D_{22}^{0})^2}
\]

It is worth noticing that, quite remarkably, the manipulations performed on \( \hat{\rho}^{(1)} \) preserve the structure of (A.29) in the final form, hence we can write

\[
\mathcal{L}^{(1)} = (i \mathcal{L}_\omega \partial_T - i \mathcal{L}_k \partial_X - i \mathcal{L}_{k\kappa} k_X + i \mathcal{L}_{\omega} \omega_T + i \mathcal{L}_{\omega k} (k_T - \omega_X) + \mathcal{L}_\epsilon), \quad (A.33)
\]

where the operators are defined as

\[
\mathcal{L} = (k \Psi_y - \omega)(-k^2 + \partial_{yy}) - k \Psi_{yy}y - \frac{gk^2 R_y}{k \Psi_y - \omega},
\]

\[
\mathcal{L}_\omega = -(-k^2 + \partial_{yy}) - \frac{gk^2 R_y}{(k \Psi_y - \omega)^2}
\]

\[
\mathcal{L}_k = \Psi_y(-3k^2 + \partial_{yy}) + 2 \omega k - \Psi_{yy}y - \frac{2gk R_y}{k \Psi_y - \omega} + \frac{gk^2 \Psi_y R_y}{(k \Psi_y - \omega)^2}
\]

\[
\mathcal{L}_\epsilon = i \Psi_X \partial_y (-k^2 + \partial_{yy}) - i \Psi_{yy} \partial_y - \frac{igk R_X}{k \Psi_y - \omega} \partial_y + \frac{igk^2 R_y \Psi_X}{(k \Psi_y - \omega)^2} \partial_y
\]

\[
\mathcal{L}_{k\kappa} = -6(k \Psi_y - 2 \omega) - \frac{2g R_y}{(k \Psi_y - \omega)} + \frac{4gk R_y \Psi_y}{(k \Psi_y - \omega)^2} - \frac{2gk^2 R_y \Psi_y^2}{(k \Psi_y - \omega)^3}
\]

\[
\mathcal{L}_{\omega k} = 2k - \frac{2gk R_y}{(k \Psi_y - \omega)^2} + \frac{2gk^2 R_y \Psi_y}{(k \Psi_y - \omega)^3}
\]

A.2.2 Discrete part: interface conditions

The boundary conditions for the inner-layer problem derive from imposing the continuity of (A.7)-(A.8) at O(1), and of (A.9)-(A.10) at O(\( \epsilon \)). Here we develop the calculations that finally lead to the boundary forms inside (A.17) and (A.19). We assume
the notation

$$\Delta_j f = f(N_j^+) - f(N_j^-) = s_j(f_M - f_j), \quad \text{with} \quad s_j = (-1)^j$$

to denote the jump of a quantity $f$ across the $j$ interface, with the convention to subtract the lower value from the upper one. The $O(1)$ interface conditions can then be expressed as

$$\Delta_j \psi^{(0)}, \quad \Delta_j p_x^{(0)} = 0. \quad (A.35)$$

In terms of the streamfunction, the first of the above conditions is just equivalent to the continuity of $\hat{\psi}^{(0)}$

$$\Delta_j \hat{\psi}^{(0)} = 0.$$  

After using the equation of motion (A.4), the second one of (A.35) becomes

$$(kU - \omega)\Delta_j \hat{\psi}^{(0)}_y - k\hat{\psi}^{(0)} \Delta_j U_y = 0. \quad (A.36)$$

Since $\hat{\psi}^{(0)}_j$ satisfies the leading-order Laplace equation

$$(\partial_{yy} - k^2)\hat{\psi}^{(0)}_j = 0 \quad (A.37)$$

it follows that $\hat{\psi}^{(0)}_j = Ae^{s_jk(y - N_j)}$, with $A = \hat{\psi}^{(0)}_M(N_j, X, T)$ for continuity. Hence, at the interface $y = N_j$, $\hat{\psi}^{(0)}_{jy}$ and $\hat{\psi}^{(0)}_M$ are related by

$$\hat{\psi}^{(0)}_{jy} = s_j k \hat{\psi}^{(0)}_j = s_j k \hat{\psi}^{(0)}_M.$$
By using this inside (A.36), we obtain closed boundary conditions for the intermediate-layer problem:

\[
(kU - \omega) \left( -k \hat{\psi}_M^{(0)} + s_j \hat{\psi}^{(0)}_{M,y} \right) - s_j k U_y \hat{\psi}^{(0)}_M = 0 \quad \text{at} \quad y = N_j.
\]

These can be recognized to be the boundary conditions of problem (A.16).

At \( O(\epsilon) \) the interfacial conditions are

\[
\Delta_j (v^{(1)} - u^{(0)} N_j X) = 0, \quad \Delta_j (p_x^{(1)} + p_x^{(0)} + p_y^{(0)} N_j X) = 0, \quad (A.38)
\]

after using (A.5), (A.6) and the ansatz (A.13), the above equations become

\[
\Delta_j \left( i k \hat{\psi}^{(1)} + \hat{\psi}_x^{(0)} + \hat{\psi}_y^{(0)} N_j X \right) = 0, \quad (A.39)
\]

\[
\Delta_j \left( -i \omega \hat{\psi}_y^{(1)} + \hat{\psi}_{yT}^{(0)} + i k U \hat{\psi}_y^{(1)} + U \hat{\psi}_y^{(0)} - U_y \hat{\psi}_X^{(0)} - i k U_y \hat{\psi}^{(1)} + U_X \hat{\psi}_y^{(0)} + N_j X U \hat{\psi}_{yy}^{(0)} \right) = 0. \quad (A.40)
\]

In order to obtain a closed internal-layer problem we need to express \( \Delta_j \hat{\psi}^{(1)} \) and \( \Delta_j \hat{\psi}_{y}^{(1)} \) in terms of \( \hat{\psi}_M^{(1)} \) and quantities determined at the previous order.

For a function \( f(X, y) \) continuous across \( N_j \) the component of the gradient tangent to the interface must also be continuous, i.e., \( \Delta_j f_X + N_j f_y = 0 \), hence equation (A.39) implies

\[
\Delta_j \hat{\psi}^{(1)} = 0. \quad (A.41)
\]

In order to manipulate \( \Delta_j \hat{\psi}_{y}^{(1)} \) we need to consider first the outer-layer solutions. In the outer layers (A.32) expresses the conservation of \( O(\epsilon) \)-vorticity by leading-order flow advection:

\[
(k \Psi_y - \omega) (\nabla^2 \hat{\psi}_j^{(1)}) = 0 \quad (A.42)
\]

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For \((k\Psi_y - \omega) \neq 0\) this implies

\[
(\nabla^2 \hat{\psi}_j)^{(1)} = \psi^{(1)}_{jyy} - k^2 \psi^{(1)}_j + 2ik\psi^{(0)}_{jX} + ikX\psi^{(0)}_j = 0. \tag{A.43}
\]

For such differential equation, the homogeneous and particular solution vanishing at infinity are

\[
\hat{\psi}_h(y, X) = e^{s_jk(y - N_j)}
\]

and

\[
\hat{\psi}_p(y, X) = -s_j(y - N_j) \left( i\hat{\psi}^{(0)}_{jX} + ik\hat{\psi}^{(0)}_j / 2k \right),
\]

respectively. By observing that \(\hat{\psi}_p(N_j, X) = 0\), so that \(\hat{\psi}^{(1)}_j(N_j, X) = \hat{\psi}_h(N_j, X)\), it follows

\[
\begin{align*}
\Delta_j \hat{\psi}^{(1)}_y &= s_j \left( \hat{\psi}^{(1)}_M - \hat{\psi}^{(1)}_{jy} \right) \\
&= s_j \left( \hat{\psi}^{(1)}_M - \hat{\psi}^{(1)}_{jy} \right) \\
&= s_j \hat{\psi}^{(1)}_M - k\hat{\psi}^{(1)}_M - iN_jX \left( \hat{\psi}^{(0)}_M - \hat{\psi}^{(0)}_j \right)
\end{align*}
\]

at \(y = N_j\), hence

\[
\Delta_j \hat{\psi}^{(1)}_y = s_j \left( \hat{\psi}^{(1)}_M - \hat{\psi}^{(1)}_{jy} \right) = s_j \hat{\psi}^{(1)}_M - k\hat{\psi}^{(1)}_M + iN_jXkU_y\hat{\psi}^{(0)}_M / (kU_j - \omega).
\]

We next need to notice the identities

\[
\begin{align*}
\Delta_j \hat{\psi}^{(0)}_y = s_j \hat{\psi}^{(0)}_M - \left( k\hat{\psi}^{(0)}_{jX} + kX\hat{\psi}^{(0)}_j \right) \\
&= s_j \hat{\psi}^{(0)}_M - \left( k\hat{\psi}^{(0)}_{jX} + N_Xk\hat{\psi}^{(0)}_M - s_jk^2N_X\hat{\psi}^{(0)}_M + kX\hat{\psi}^{(0)}_M \right),
\end{align*}
\]

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and

\[ \Delta_j \hat{\psi}_y^{(0)} = s_j \hat{\psi}_{My}^{(0)} - (k \hat{\psi}_M^{(0)} + k_T \hat{\psi}_M^{(0)}) \]

which, together with (A.41), are used in (A.40).

This completes the preliminaries needed to simplify of (A.40), which can be now written as

\[ i(kU_j - \omega) \Delta_j \hat{\psi}_y^{(1)} - i k \Delta_j U_y \hat{\psi}_M^{(1)} \]

\[ + \Delta_j \hat{\psi}_y^{(0)} + U_j \Delta_j \hat{\psi}_x^{(0)} - (\Delta_j U_y \hat{\psi}_{MX}^{(0)} + U_y \Delta_j \hat{\psi}_x^{(0)} - s_j \Delta_j U_y \Delta_j \hat{\psi}_x^{(0)}) \]

\[ + (U_{MX} \Delta_j \hat{\psi}_y^{(0)} + \Delta_j U_X \hat{\psi}_{My}^{(0)} - s_j \Delta_j U_X \Delta_j \hat{\psi}_y^{(0)}) + N_{jX} U_j \Delta_j \hat{\psi}_{yy}^{(0)} = 0. \]

Using \( \Delta_j U_X = -N_{jX} \Delta_j U_y = -N_{jX} s_j U_y \) and \( U_{MX} = U_{jX} - N_{jX} U_y \), we expand all increments and obtain

\[ i(kU_j - \omega) \left( s_j \hat{\psi}_{My}^{(1)} - k \hat{\psi}_M^{(1)} + i N_{jX} k U_y \hat{\psi}_M^{(0)} / (kU_j - \omega) + i \hat{\psi}_{MX}^{(0)} \right) \]

\[ -i k s_j U_y \hat{\psi}_M^{(1)} + \left[ s_j \hat{\psi}_{My}^{(1)} - \left( k \hat{\psi}_M^{(0)} + k_T \hat{\psi}_M^{(0)} \right) \right] \]

\[ + U_j \left[ s_j \hat{\psi}_{My}^{(0)} - \left( k \hat{\psi}_M^{(0)} + N_{jX} k \hat{\psi}_{My}^{(0)} - s_j k^2 N_{jX} \hat{\psi}_M^{(0)} + k_X \hat{\psi}_M^{(0)} \right) \right] \]

\[ - s_j U_y \hat{\psi}_M^{(0)} \]

\[ + U_{jX} \left( s_j \hat{\psi}_{My}^{(0)} - k \hat{\psi}_M^{(0)} \right) - N_{jX} s_j U_y \hat{\psi}_M^{(0)} + N_{jX} U_j s_j \left( \hat{\psi}_{My}^{(0)} - k^2 \hat{\psi}_M^{(0)} \right) = 0. \]
Some further manipulations the above equation becomes

\[
\begin{align*}
&i s_j (k u_j - \omega) \hat{\psi}_{My}^{(1)} - i k (k u_j - \omega) \hat{\psi}_M^{(1)} - i k s_j u_y \hat{\psi}_M^{(1)} = \\
&\quad -s_j \psi_{MyT}^{(0)} + k \psi_{MT}^{(0)} \\
&\quad + (s_j u_y + 2 k u_j - \omega) \psi_{MX}^{(0)} - s_j \psi_{MyX}^{(0)} \\
&\quad + (U_j X k + N_{jX} k u_y) \psi_M^{(0)} - (s_j U_{jX} - N_{jX} k u_j - s_j N_{jX} u_y) \psi_{My}^{(0)} - s_j N_{jX} U_{jy} \hat{\psi}_{My}^{(0)} \\
&\quad + U_j k \hat{\psi}_M^{(0)} + k T \hat{\psi}_M^{(0)} \\
&\quad \hat{\psi}_{Mk}^{(0)} + \hat{\psi}_{\omega k}^{(0)}
\end{align*}
\]

(A.44)

where in the last step we used again (A.36) on the second term containing the factor \(N_X\). In the above expression one can precisely identify the boundary conditions of problem (A.17).

A.3 A few useful relations

A.3.1 Computing \(\Omega_k\) and \(\Omega_X\) from eigenfunctions

Let \(\mathcal{L}\) be a linear operator that depends on the parameters \(k\), \(\omega\), and \(X\), and \(\phi\) an eigenfunction for the eigenvalue problem

\[
\mathcal{L}[k, \omega, X] \phi = 0, \quad U[k, \omega, X] \phi = 0.
\]

(A.45)
The parameter regarded as the eigenvalue is $\omega$, which then depends on the other two through the dispersion relation $\omega = \Omega(k, X)$. Assume the expansion of $\phi$ in $k$ about $k_0$

$$\phi = \phi_0 + (k - k_0)\phi_k + \frac{1}{2}(k - k_0)^2\phi_{kk} + \ldots$$

and differentiate problem (A.45) in $k$ about $k = k_0$ to obtain a problem in $\phi_k$

$$L_0\phi_k + L_k\phi_0 + \Omega_k\phi_0 = 0,$$

$$U_0\phi_k + U_k\phi_0 + \Omega_k\phi_0 = 0,$$

where the differentiated operators operators appear. After taking the inner product of the above boundary value problem with the solution of the associated adjoint-homogeneous problem (i.e. summing the pairing of differential and boundary form parts as in the solvability condition (A.20)), and using the fact that $$(L\phi_k, \phi_0^\dagger) - U_k\phi_0 \cdot U_0^\dagger \phi_0^\dagger = 0,$$

we obtain

$$\Omega_k = -\frac{(L_k\phi_0, \phi_0^\dagger) - U_k\phi_0 \cdot U_0^\dagger \phi_0^\dagger}{(L_\omega\phi_0, \phi_0^\dagger) - U_\omega\phi_0 \cdot U_0^\dagger \phi_0^\dagger} \quad (A.46)$$

One can proceed in a similar manner perturbing the eigenvalue problem with respect to $X$, and obtain

$$\Omega_X = -\frac{(L_X\phi_0, \phi_0^\dagger) - U_X\phi_0 \cdot U_0^\dagger \phi_0^\dagger}{(L_\omega\phi_0, \phi_0^\dagger) - U_\omega\phi_0 \cdot U_0^\dagger \phi_0^\dagger} \quad (A.47)$$

### A.3.2 Adjoint boundary form

In this section we report the details regarding the solvability condition (A.20) for boundary value problems encountered in §A.1.

Let $L$ and $L^\dagger$ be a second order linear operator and its adjoint. Considering any two complex-valued functions $u$ and $v$ defined on a $[a, b]$ real interval, the following relation
holds identically (Coddington & Levinson [30]):

$$
(Lu,v) - (u,L^tv) = \left. u'v'^\dagger \right|_a^{b} - \left. uv'^\dagger \right|_a^{b} \\
= [uv](a) - [uv](b),
$$

(A.48)

where

$$
[uv](y) = B_{jk}u^{(k-1)}(y)v^{(k-1)}(y),
$$

(A.50)

with

$$
B = \begin{bmatrix}
0 & 1 \\
-1 & 0
\end{bmatrix}.
$$

Consider a boundary value problem on $[a,b]$

$$
Lu = f, \quad Uu = b,
$$

where the boundary conditions are expressed in the boundary form notation. The boundary form $Uu$ is a short-hand notation for the matrix-vector product

$$
[U] \bar{u}
$$

where $\bar{u} = [u(a) u'(a) u(b) u'(b)]$, and $[U]$ is the matrix expressing the desired boundary conditions. The formula (A.48) is related to the boundary forms by the following boundary-form formula (BFF) (page 288 on Coddington & Levinson’s book)

$$
[uv](a) - [uv](b) = Uu \cdot U^\dagger v + U_e u \cdot U^\dagger v.
$$

Considering $U$ known, and the corresponding $U^\dagger$ defined in the natural way (by the matrix $[U^\dagger]$ being the transposed-conjugate of $[U]$), the above formula represents a
definition of the two associated complementary boundary forms.

Let $\xi$ be an eigenfunction of the adjoint boundary value problem

$$ L^\dagger \xi = 0, \quad U^\dagger \xi = 0. $$

For $v = \xi$ the BFF reduces to

$$ [u\xi](a) - [u\xi](b) = Uu \cdot U^\dagger v. $$

By using (A.50), we can adopt an explicit matrix notation and rewrite the above formula as

$$ \pi^T \tilde{B} \bar{\xi} = \pi^T [\mathcal{U}]^T [\mathcal{U}^\dagger] \bar{\xi}. \quad (A.51) $$

where

$$ \tilde{B} = \begin{bmatrix} B & 0 \\ 0 & B \end{bmatrix}. $$

Since $u$ is arbitrary, (A.51) implies

$$ \tilde{B} \bar{\xi} = [\mathcal{U}]^T [\mathcal{U}^\dagger] \bar{\xi}, $$

and after pre-multiplying by $[\mathcal{U}]$ we obtain

$$ [\mathcal{U}] \tilde{B} \bar{\xi} = [\mathcal{U}] [\mathcal{U}]^T [\mathcal{U}^\dagger] \bar{\xi}, $$

which is a $4 \times 4$ linear system in $[\mathcal{U}^\dagger] \bar{\xi}$, that determines the form $\mathcal{U}^\dagger \xi$ necessary to impose the solvability condition (A.20).
Appendix B

SCALAR VARIANCE EVOLUTION FROM TAYLOR MODES
(APPENDIX TO PART II)

In this appendix it is reported an exact calculation for the scalar variance evolution based on the Taylor modes, as defined in § 8.2. This derivation is an alternative approach leading to the same results obtained by Camassa et al.[21] using SDE analysis. Quite remarkably, information on the full time evolution is contained in the class of eigemodes connected to the Taylor (hence long-time) regime.

B.1 Problem Formulation

We consider initial value problems for the advection-diffusion equation

\[ T_t + (u \cdot \nabla) T = P e^{-1} \nabla^2 T, \]  
(B.1)

with vanishing Neumann (insulating) condition at the boundaries, and assigned parallel flow \( u = u \hat{x} \). The initial condition is denoted by

\[ T|_{t=0} = T_0(x). \]

We consider both the geometries of plane channel flow and circular pipe flow, the flow profiles respectively are

\[ u(y) = y^2 - 1/3, \quad y \in [-1, 1] \quad \text{for plane channel} \]
\[ u(r) = r^2 - 1/2, \quad r \in [0, 1] \quad \text{for circular pipe} \]
The natural choice of coordinates is understood in both cases, notice that we are working in a system of reference in which the average flow speed is null.

It is assumed an non-dimensionalization based on the characteristic velocity scale $U$ of $u$, and of the transversal extension of the domain as the lengthscale $L$. The nondimensional diffusion coefficient is the inverse of the Peclét number $Pe = UL/\kappa$, where $\kappa$ is the dimensional diffusivity of the scalar. The velocity field is considered to be a parallel shear layer with velocity directed along $x$ dependent from $y$.

### B.2 Eigenvalue problem, perturbative analysis

The solution $T$ is expressed as a Fourier integral in the streamwise $x$ direction, as in (7.2), then each $y$-dependent Fourier coefficient is further expanded on the eigenfunction basis

$$\hat{T}(k, y, t) = \sum_{n=0}^{+\infty} A_n(\delta)\psi_n(y, \delta)e^{kc_n t - Pe^{-1}k^2 t}$$

where $\delta = 1/(kPe)$ is the only parameter the unknown quantities depend from, and the amplitudes $A_n$ are given by projecting the (Fourier transformed) initial data $\hat{T}_0$ on the eigenfunctions $\psi_n^\dagger$ of the adjoint problem

$$A_n = \frac{\left(\hat{T}_0, \psi_n^\dagger\right)}{\left(\psi_n, \psi_n^\dagger\right)}$$

with inner-product defined as

$$\left(f, g\right) = \int_{-1}^{1} fg^*dy, \quad \text{Plane Channel;}$$

$$\int_{0}^{1} rf g^*dr, \quad \text{Circular Pipe.}$$
The pairs \((\psi_n, c_n)\) are solutions of the eigenvalue problem

\[
\mathcal{L}[c_n, \delta] \psi_n = iu(y) \psi_n, \quad \frac{d\psi_n}{dy}(a) = \frac{d\psi_n}{dy}(b) = 0
\] (B.4)

depending on the parameter \(\delta\), where the linear operator \(\mathcal{L}[c_n, \delta]\) is defined as

\[
\mathcal{L}[c_n, \delta] = \delta \frac{d^2}{dy^2} - c_n, \quad \text{Plane Channel}
\]
\[
= \delta \frac{d^2}{dr^2} + \delta \frac{1}{r} \frac{d}{dr} - c_n, \quad \text{Circular Pipe.}
\] (B.5)

The following regular expansions in \(\delta\) are assumed

\[
\psi_n = \sum_{j=0}^{+\infty} \delta^{-j} \psi_{nj}, \quad c_n = \sum_{j=0}^{+\infty} \delta^{-j+1} c_{nj}, \quad A_n = \sum_{j=0}^{+\infty} \delta^{-j} A_{nj}
\] (B.6)

with the normalization

\[
(\psi_{n0}, \psi_{n0}^\dagger) = 1,
\] (B.7)

and the additional condition

\[
(\psi_n(\delta), 1) = (\psi_0, 1),
\]

needed to determine without ambiguity the \(\delta\)-parametrized family of functions \(\psi\) in that, for any \(g(\delta)\), any family \(g(\delta) \psi(\delta)\) would be a correctly posed choice.

The eigenfunctions \(\psi_{nj}\)'s are determined by the hierarchy of equations

\[
O(\delta): \quad \mathcal{L}[c_{n0}, 1] \psi_{n0} = 0,
\]
\[
O(1): \quad \mathcal{L}[c_{n0}, 1] \psi_{n1} = (c_{n1} + iu(y)) \psi_{n0},
\]
\[
\vdots
\]
\[
O(\delta^{1-m}): \quad \mathcal{L}[c_{n0}, 1] \psi_{nm} = (c_{n1} + iu(y)) \psi_{nm-1} + \sum_{p=1}^{m-1} c_{np+1} \psi_{nm-p-1}.
\]
At leading-order the solution to the problem results trivial for both the channel and pipe flows. At the higher orders a solvability condition on the right-hand side determines the higher-order correction to \( c_n \).

At \( O(1) \) the orthogonality condition is given by

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

which expresses the physical fact that Taylor modes possess a phase speed which is the mean flow velocity at leading order. At \( O(\delta^{-1}) \) solvability condition is

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

Notice that \( c_{02} \) is the Taylor constant (i.e., effective diffusivity) for a given shear profile \( u(y) \).

The coefficients in the expansion for the \( A_n \)’s are obtained expanding numerator and denominator in (B.3), in particular, the first three terms are

\[
A_{n0} = \left( \hat{T}_0, \psi_{n0}^\dagger \right),
\]

\[
A_{n1} = \left( \hat{T}_0, \psi_{n1}^\dagger \right) - \left( \hat{T}_0, \psi_{n0}^\dagger \right) \left[ \psi_{n0}, \psi_{n1} \right],
\]

\[
A_{n2} = \left( \hat{T}_0, \psi_{n2}^\dagger \right) - \left( \hat{T}_0, \psi_{n1}^\dagger \right) \left[ \psi_{n0}, \psi_{n1} \right] + \left( \hat{T}_0, \psi_{n0}^\dagger \right) \left[ \psi_{n0}, \psi_{n1} \right]^2

+ \left( \hat{T}_0, \psi_{n0}^\dagger \right) \left[ \psi_{n0}, \psi_{n1}, \psi_{n2} \right],
\]

where the square bracket operator is defined as

\[
[\psi_{n0}, \psi_{n1}, ..., \psi_{nm}] = (\psi_{nm}, \psi_{n0}^\dagger) + (\psi_{nm-1}, \psi_{n1}^\dagger) + ... + (\psi_{n0}, \psi_{nm}^\dagger).
\]

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B.3 Longitudinal dispersion

In what follows we move the focus on cross-section-averaged quantities, henceforth denoted with an overbar \( \overline{\cdot} \). Cross averages yield condensed representations for the evolution of \( T \) in the streamwise direction. The averaging operator can be expressed in terms of inner product

\[
\overline{g} = b(g, 1)
\]

with

\[
b = \begin{cases} 
1/2 & \text{for plane channel} \\
2 & \text{for circular pipe} 
\end{cases}
\]

The \( n^{th} \)-order moments \( M_n \) of a distribution \( D(x) \) are related to its Fourier transform \( \hat{D}(k) \) by the well-known relations

\[
M_n(t) = i^n \left. \frac{\partial^n \hat{D}}{\partial k^n} \right|_{k=0},
\]

using the moments of \( \overline{T}(x, t) \) we define the effective streamwise diffusivity experienced by the passive scalar

\[
\kappa_{\text{eff}} \equiv \frac{M_2(t) - M_1(t)^2}{t}. \tag{B.12}
\]

The calculation of such quantity is the main goal in the remainder of this chapter.

The expansion for \( \hat{T}(k, t) \) is obtained just by averaging the expansion (B.2) term-by-term

\[
\hat{T} = \sum_{n=0}^{+\infty} A_n \overline{\psi}_n e^{k_n t} - Pe^{-1} k^2 t. \tag{B.13}
\]

In order to compute the first two \( x \)-moments of \( \hat{T} \) one can use the above \( \delta \)-expansion on (B.13), and retain the minimal number of terms necessary to evaluate the first two
derivatives in $k$ of $\hat{T}$ at $k = 0$ consistently:

$$\hat{T} \sim \sum_{n=1}^{+\infty} \left( A_{n0} + \delta^{-1} A_{n1} + \delta^{-2} A_{n2} \right) \left( \overline{\psi}_{n0} + \delta^{-1} \overline{\psi}_{n1} + \delta^{-2} \overline{\psi}_{n2} \right) e^{(\delta c_{n0} + c_{n1} + \delta^{-1} c_{n2})k - Pe^{-1}k^2} e^{[\delta c_{n0} + c_{n1} + \delta^{-1} c_{n2})k - Pe^{-1}k^2]t}. \tag{B.14}$$

After a tedious yet straight-forward calculation it is obtained

$$\frac{\partial \hat{T}}{\partial k} \bigg|_{k=0} = PeA_{01}\overline{\psi}_{00} + \sum_{n=1}^{+\infty} \frac{1}{Pe^{-1}A_{n0}} \overline{\psi}_{n1} e^{Pe^{-1}c_{n0}t}, \tag{B.15}$$

$$\frac{\partial^2 \hat{T}}{\partial k^2} \bigg|_{k=0} = 2Pe^2A_{02}\overline{\psi}_{00} + 2A_{00}\overline{\psi}_{00} \left( c_{02}Pe - Pe^{-1} \right) t + \sum_{n=1}^{+\infty} \left[ A_{n1}\overline{\psi}_{n1} + A_{n0}(Pe^{-1}c_{n1}\overline{\psi}_{n1}t + \overline{\psi}_{n2}) \right] 2e^{Pe^{-1}c_{n0}t} Pe^2. \tag{B.16}$$

These relations are so far general, in that no specific choice of initial data or velocity profile has been assumed. In what follows we are going to work out explicit results for particular cases.

### B.3.1 Channel flow with transversely uniform data

We fix now the choice $u(y) = y^2 - 1/3$ and $T(x, y, t)|_{t=0} = \delta(x)$ which corresponds to initial data uniform along the cross section and concentrated in the streamwise direction. In this case the calculation of any term needed in (B.16)-(B.15) can be worked explicitely.

The easy solution of the leading-order problem results to be

$$\psi_{n0} = \cos(n\pi y), \quad c_{n0} = -\pi^2 n^2, \quad (n > 0)$$

$$= \frac{1}{\sqrt{2}}, \quad = 0, \quad (n = 0) \tag{B.17}$$

The solution up to $O(\delta^{-1})$ of the eigenvalue problem for $\psi_{0}, c_0$ is required to find $c_{02}$. 191
At $O(1)$ the equation reads
\[ \frac{d^2 \psi_{01}}{dy^2} = (c_{01} + i(y^2 - 1/3))\psi_{00}, \]
and condition (B.8) gives $c_{01} = 0$ (since we assigned a mean-zero velocity profile). We then find
\[ \psi_{01} = i(y^4/12 - y^2/6 + 7/180)\psi_{00}. \]

At $O(\delta^{-1})$ we have
\[ \frac{d^2 \psi_{02}}{dy^2} = -(y^2 - 1/3)(y^4/12 - y^2/6 + 7/180)\psi_{00} + c_{02}\psi_{00}, \]
using condition (B.9) we obtain $c_{02} = -8/945$, which is the known value of the Taylor constant for the channel flow.

The initial condition implies $\hat{T}_0(k, y) = 1$, hence from (B.17) and (B.10) we obtain $A_{n0} = 0$ if $n \neq 0$ and $A_{00} = \sqrt{2}$. Being $\psi_{00}$ constant and $\psi_{01}^\dagger$ a mean-zero function we have $A_{01} = 0$. Considering again the zero-mean property of the non-leading-order terms in the expansion of $\psi_0$ we see that the expression for $A_{02}$ reduces to
\[ A_{02} = (1, \psi_{00}^\dagger) (\psi_{01}, \psi_{01}^\dagger) = \int_{-1}^{1} (y^4/12 - y^2/6 + 7/180)^2 dy = \frac{8}{9450\sqrt{2}}. \]

The expression for $A_{n1}$ reduces to
\[ A_{n1} = (1, \psi_{n1}^\dagger) = \int_{-1}^{1} \psi_{n1}^\dagger dy = \int_{-1}^{1} \frac{i\psi_{n0}^\dagger}{c_n} dy = (-1)^n \frac{4i}{\pi^4 n^4}, \quad n > 0, \]
using the adjoint equation satisfied by $\psi_{n1}^\dagger$. Similarly we have $\overline{\psi_{n1}} = A_{n1}/2, \quad n > 0$. 

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Finally, the specific form of (B.15) and (B.16) for this case results to be

\[
\frac{\partial \hat{T}}{\partial k}
\Bigg|_{k=0} = 0, \tag{B.18}
\]

\[
\frac{\partial^2 \hat{T}}{\partial k^2}
\Bigg|_{k=0} = \left( \frac{8}{945} Pe - 2 Pe^{-1} \right) t + 8 Pe^2 \left( \frac{1}{9450} - \sum_{n=1}^{\infty} \frac{e^{-Pe^{-1} \pi^2 n^2 t}}{\pi^8 n^8} \right). \tag{B.19}
\]

### B.3.2 Pipe flow with transversely uniform data

Now we work in cylindrical coordinates, the steady velocity profile for the Poiseuille flow is given by

\[ u(r, \theta, x) = r^2 - 1/2, \]

again, it is chosen a reference system that makes the mean flow speed to be null. The initial data is uniformly distributed along the pipe section, namely

\[ T(r, \theta, x, t)|_{t=0} = \delta(x). \]

The \( O(\delta) \) problem in the \( \delta \)-expansion is a (zeroth-order) Bessel equation. The solution, normalized according to (B.7), consists of

\[
\psi_{n0} = \sqrt{2} \frac{J_0(\mu_n r)}{J_0(\mu_n)}, \quad c_{n0} = -\mu_n^2, \quad \text{for } n > 0 \]

\[ = \sqrt{2}, \quad = 0, \quad \text{for } n = 0. \tag{B.20} \]

In the above formula \( \mu_n > 0 \) is defined by \( J_1(\mu_n) = -J'_0(\mu_n) = 0 \). Proceeding to the higher orders we find at \( O(1) \)

\[ \psi_{01} = i(r^4/16 - r^2/8 + 1/24) \psi_{00}, \]

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and at $O(\delta^{-1})$

$$\mathcal{L}[c_{n0}, 1]\psi_{n2} = -(r^2 - 1/2)(r^4/16 - r^2/8 + 1/24)\psi_{00} + c_{02}\psi_{00}.$$  

Condition (B.9) yields $c_{02} = -1/192$. By repeating the same procedure as for the plane channel flow, we now obtain

$$A_{00} = 1/\sqrt{2},$$

$$A_{01} = 0,$$

$$A_{02} = 1/5760/\sqrt{2},$$

$$A_{n0} = 0, \quad n > 0,$$

$$A_{n1} = \frac{i2\sqrt{2}}{\mu^4_n}, \quad n > 0,$$

$$\psi_{n1} = \frac{i4\sqrt{2}}{\mu^4_n}, \quad n > 0,$$

and

$$\left.\frac{\partial \hat{T}}{\partial k}\right|_{k=0} = 0,$$

$$\left.\frac{\partial^2 \hat{T}}{\partial k^2}\right|_{k=0} = -2\left(\frac{1}{192Pe^{-1} + Pe^{-1}}\right)t + \frac{1}{Pe^{-2}} \left(\frac{2}{5760} - 32 \sum_{n=1}^{\infty} e^{-Pe^{-1}}\frac{\mu^8_n}{\mu^n_n}t\right).$$


