A statistical mechanics theory for mixing in stratified fluids

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Abstract

Predicting how much mixing occurs when a given amount of energy is injected into a Boussinesq fluid is a longstanding problem in stratified turbulence. Here we address this problem with the point of view of equilibrium statistical mechanics. Assuming random evolution through turbulent stirring, the theory predicts that the unforced, inviscid, adiabatic dynamics is attracted irreversibly towards a state characterised by wild small scale velocity fluctuations carrying kinetic energy, and by a smooth buoyancy profile superimposed with wild small scale buoyancy fluctuations. It is then possible to compute how much of the injected energy has been irreversibly lost into small scale kinetic energy, the remaining part being used to irreversibly raise the potential energy of the system. This yields to quantitative predictions for a global, cumulative mixing efficiency in freely evolving configurations. We argue that this approach may be useful to the understanding of mixing in stratified turbulence in the limit of large Reynolds and Péclet numbers.

1 Introduction

The large-scale stratification and dynamics of the oceans depend crucially on localised turbulent mixing events (Wunsch and Ferrari, 2004). These mixing processes occur on temporal and spatial scales much smaller than the current resolutions of general circulation models and must therefore be parameterised (Large et al., 1994). It is essential for that purpose to know how much mixing occurs when stratification is stirred by a turbulent flow (Hopfinger, 1987; Peltier and Caulfield, 2003; Ivey et al., 2008). More precisely, which fraction of the injected energy is lost through a direct turbulent kinetic energy cascade, which fraction contributes to modifying the background stratification, and what is the resulting vertical buoyancy profile? Building upon previous work by Tabak and Tal (2004), we propose here to use equilibrium statistical mechanics as a guideline to answer those questions (Venaille et al., 2016)

The traditional approach to estimate the efficiency of mixing in stratified turbulence involves direct analyses of the diffusive destruction of small scale buoyancy variance, which in turn requires a separation of the influence of stirring from that of irreversible mixing through application of the Lorenz concept of available potential energy that can be converted into kinetic energy and a base-state potential energy which can not (Winters et al., 1995). The diffusive destruction of small scale buoyancy variance may be represented by the time derivative $\mathcal{M}$ of base-state potential energy plus a small correction due to the action of molecular diffusion on the initial stratification, a correction that become negligible in the limit of high Reynolds number. The time dependent efficiency of turbulent mixing may then be computed from direct numerical or laboratory experiments as $\eta_{inst} = \mathcal{M}/(\mathcal{M}+\epsilon)$ where ϵ is the viscous dissipation of kinetic energy in the flow; see e.g. (Peltier and Caulfield, 2003). This definition of mixing efficiency is global in space since

the computation of the base-state potential energy requires a rearrangement of the fluid particle at the domain scale. Using a number of additional assumptions, it may be related to a local mixing efficiency that is often used in oceanography to model an effective diffusivity for diapycnal mixing Osborn (1980); Hopfinger (1987). In decaying experiments, it is also convenient to define a cumulative mixing efficiency $\eta = \int_0^{+\infty} \mathrm{d}t \mathcal{M} / \int_0^{+\infty} \mathrm{d}t \, (\mathcal{M} + \epsilon)$, which measures how much of the total injected energy has been used to irreversibly raise the potential energy of the flow in the experiment.

Equilibrium statistical mechanics counts the available states of an isolated physical system with given constraints based on conservation laws. Under random evolution, the system is expected to reach the *macroscopic* state which corresponds to the maximum number of *microscopic* configurations. In this paper, the *macroscopic* quantity to be determined by the theory is the partition between kinetic and potential energy, as well as the corresponding mean (coarse-grained) vertical buoyancy profile. The *microscopic* configurations will be any buoyancy field and non-divergent velocity field, and the constraints will be provided by dynamical invariants of the flow model. The equilibrium statistical mechanics theory applies to the freely evolving inviscid adiabatic dynamics. Considering such an approach to describe actual stratified turbulence amounts to assuming that the Reynolds number Re and the Péclet number Pe are sufficiently large, and that the typical time scale to reach the equilibrium state is smaller than the typical time scale associated with molecular viscosity and diffusivity.

In order to compute the equilibrium state associated with a given initial configuration, one only needs to know the dynamical invariants, which are the total energy and the global distribution of buoyancy levels. The theory predicts that some part of the initial energy is irreversibly lost into small scales kinetic energy, which can be computed explicitly. This makes possible predictions for a cumulative mixing efficiency in the framework of an inviscid, adiabatic flow model.

The equilibrium statistical mechanics theory is presented in the second section. Application to the computation of mixing efficiency is presented in a third section, which includes a discussion on irreversibility for an inviscid, adiabatic fluid. We provide predictions for the variation of mixing efficiency with the bulk Richardson number, and show that such variations depend strongly on the initial buoyancy profile. A discussion and a summary of the main results is given in a fourth section.

2 Equilibrium statistical mechanics of non-rotating Boussinesq fluids

We consider an inviscid Boussinesq fluid that takes place in a three-dimensional domain $\mathcal{V}_{\mathbf{x}}$ of volume V. Spatial coordinates are denoted $\mathbf{x} = (x, y, z)$, with $\mathbf{e}_z$ the vertical unit vector pointing in the upward direction. At each time t the system is described by the buoyancy field $b(\mathbf{x}, t)$ and by the velocity field $\mathbf{u}(\mathbf{x}, t) = (u, v, w)$, which is non-divergent. The unforced, inviscid, adiabatic dynamics is given by

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\varrho_0} \nabla P + b \mathbf{e}_z \ , \quad \nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\partial_t b + \mathbf{u} \cdot \nabla b = 0 \ . \tag{2}$$

The first step before computing equilibrium states of this dynamical system is to define what is a *microscopic configuration* of the system, which requires to identify the relevant phase space that satisfy a Liouville theorem. This means that the flow in phase-space is non-divergent. Consequently, if all microscopic states are equiprobable at a given time,

they remain equiprobable through the flow evolution. It is shown in Venaille et al. (2016) that the quadruplet of fields $b, \mathbf{u}$ satisfies such a Liouville theorem.

The second step is to identify relevant dynamical invariants, which are here total energy and the global distribution of buoyancy levels. The ensemble of microscopic configurations characterised by the same dynamical invariants define the microcanonical ensemble. This is the relevant ensemble to be considered in the framework of an unforced, inviscid, adiabatic Boussinesq system.

The third step is to identify relevant macrostates, which describe ensembles of microstates. We introduce for that purpose the probability $\rho(\mathbf{x}, \sigma, \mathbf{v})$ of finding the buoyancy level σ and the velocity level $\mathbf{v}$ in the vicinity of point $\mathbf{x}$. The probability density field ρ is normalised at each point :

$$\forall \mathbf{x} \in \mathcal{V}_\mathbf{x},\ \mathcal{N}_\mathbf{x}[\rho] = \int_{\mathcal{V}_\mathbf{v}} \mathrm{d}\mathbf{v} \int_{\mathcal{V}_\sigma} \mathrm{d}\sigma\ \rho(\mathbf{x}, \sigma, \mathbf{v}) = 1\ , \tag{3}$$

where the integral bounds are

$$\mathcal{V}_\mathbf{v} = [-\infty,\ +\infty]^3\,, \quad \mathcal{V}_\sigma = [-\infty,\ +\infty]\,. \tag{4}$$

Each microscopic state $(b(\mathbf{x}), \mathbf{u}(\mathbf{x}))$ is described at a macroscopic level by the pdf $\rho(\mathbf{x}, \sigma, \mathbf{v})$, which can be interpreted as the local volume proportion of fluid particles carrying the buoyancy level σ and velocity level $\mathbf{v}$. Several useful macroscopic fields can be deduced from ρ, such as the macroscopic buoyancy field

$$\overline{b}(\mathbf{x}) = \int_{\mathcal{V}_\sigma} \mathrm{d}\sigma \int_{\mathcal{V}_\mathbf{v}} \mathrm{d}\mathbf{v}\ \rho\sigma\ , \tag{5}$$

and the local eddy kinetic energy field

$$\frac{1}{2}\overline{\mathbf{u}^2}(\mathbf{x}) = \int_{\mathcal{V}_\sigma} \mathrm{d}\sigma \int_{\mathcal{V}_\mathbf{v}} \mathrm{d}\mathbf{v}\ \frac{1}{2}\rho\mathbf{v}^2\ . \tag{6}$$

The interest of considering the probability field ρ for a macroscopic description of the system is that global constraints provided by dynamical invariants can be expressed in term of this quantity:

$$\mathcal{E}[\rho] = \int_{\mathcal{V}_\mathbf{x}} \mathrm{d}\mathbf{x} \int_{\mathcal{V}_\mathbf{v}} \mathrm{d}\mathbf{v} \int_{\mathcal{V}_\sigma} \mathrm{d}\sigma\ \rho \left(\frac{\mathbf{v}^2}{2} - \sigma z \right)\ , \tag{7}$$

$$\mathcal{G}_\sigma[\rho] = \int_{\mathcal{V}_\mathbf{x}} \mathrm{d}\mathbf{x} \int_{\mathcal{V}_\mathbf{v}} \mathrm{d}\mathbf{v}\ \rho\ . \tag{8}$$

The last step is to count how many microscopic configurations are associated with a given macrostate, and to show that there is a concentration of an overwhelming number of microscopic states close to the most probable macrostate in a given microcanonical ensemble (i.e. for a given set of constraints). It is shown in Venaille et al. (2016) that this most probable state maximises the entropy

$$\mathcal{S} = -\int_{\mathcal{V}_\mathbf{x}} \mathrm{d}\mathbf{x} \int_{\mathcal{V}_\mathbf{v}} \mathrm{d}\mathbf{v} \int_{\mathcal{V}_\sigma} \mathrm{d}\sigma\ \rho \ln \rho\ , \tag{9}$$

while satisfying the constraints of the problem given by Eq. (3), (7) and (8). This generalises previous results by Tabak and Tal (2004), who derived a similar expression,

but without taking into account the degrees of freedom associated with the velocity field, which was interpreted directly as a thermostat.

The variational problem of the equilibrium theory can be solved analytically in limiting cases, and solved numerically in the general case (Venaille et al., 2016). The equilibrium states are characterised by several important properties:

- The distributions of b and $\mathbf{u}$ are independent.
- The variance of velocity fluctuations and the variance of buoyancy fluctuations are proportional, and their ratio varies linearly with the local mean buoyancy gradient.
- The predicted velocity distribution is Gaussian, isotropic and homogeneous in space. It is therefore fully characterised by its variance, namely the local eddy kinetic energy

$$e_c \equiv \frac{1}{2}\overline{\mathbf{u}^2} \tag{10}$$

- The predicted buoyancy distribution $\rho_b(z,\sigma)$ depends only on the height coordinate z. The equilibrium theory predicts therefore that the local fluctuations of buoyancy are invariant on the horizontal.

3 Application: computation of mixing efficiency in decaying flows

Assuming that the equilibrium state is known (which can always be done numerically), it is possible to compute a cumulative mixing efficiency within this framework. In order to introduce a relevant definition of mixing efficiency in the context of an inviscid, adiabatic flow system, we need to consider two essential results stemming from the equilibrium theory. First, the most probable macrostate is an attractor for the dynamics, according to statistical mechanics predictions: convergence of microscopic configurations towards the equilibrium state is irreversible. We stress that this irreversibility is entirely due to the inertial dynamics, not to molecular processes. Second, the most probable macrostate has a peculiar structure: its buoyancy field is characterised by a smooth buoyancy profile $\overline{b}(z)$ superimposed with wild small scale buoyancy and velocity fluctuations. More precisely, the theory predicts that when performing a local coarse-graining of the microscopic buoyancy and velocity fields at a scale l, the small scale fluctuations are confined at scales smaller than the coarse-graining scale l, no matter how small the coarse-graining length scale l is, provided that the system is sufficiently close to equilibrium (Venaille et al., 2016).

Because all the kinetic energy of the equilibrium state is carried by small scale velocity fluctuations, one can say that the kinetic energy is literally lost irreversibly into small scales. Indeed, once the equilibrium is reached, the energy of those small scales fluctuations can not be used to overturn the coarse-grained buoyancy field. Similarly, the small scale buoyancy fluctuations can not be used to modify the mean buoyancy profile $\overline{b}$ once the equilibrium state is reached. In that respect, there is irreversible mixing of the buoyancy field at a coarse-grained level.

To conclude, when the system evolves from its initial configuration to the equilibrium state, the injected energy is partly lost into small scale kinetic energy carried by velocity fluctuations and partly used to mix the buoyancy field at a coarse-grained level. The coarse-grained buoyancy profile and the small scale fluctuations are decoupled when the equilibrium state is reached. This decoupling is very much similar to the effect of viscosity,

which transfers energy from the fluid motion degrees of freedom to internal heat degrees of freedom.

Let us assume that a given amount of energy denoted E_{inj} is injected into a fluid initially at rest, characterised by a sorted (or background, or base) buoyancy profile $b_s(z)$. The energy may either be injected on the form of kinetic energy through mechanical stirring or on the form of potential energy as for instance in Rayleigh-Taylor configurations. Turbulent stirring implies rearrangements of fluid parcels, which changes the initial sorted buoyancy field b_s into another buoyancy field b. Such rearrangements are necessarily associated with an increase of potential energy

$$E_p = -\int_{\mathcal{V}_\mathbf{x}} \mathrm{d}\mathbf{x} \ (b - b_s)\, z. \tag{11}$$

At equilibrium, this quantity can be expressed in term of the macroscopic buoyancy profile $\overline{b}$ which depends only on z:

$$E_p = \frac{V}{2H}\int_{-H}^{+H} \mathrm{d}z \ \left(\overline{b} - b_s\right) z \ . \tag{12}$$

The theory also predicts that the local kinetic energy e_c is uniform in space once the equilibrium is reached. The total kinetic energy is $E_c = V e_c$, and the conservation of energy leads to :

$$E_p + E_c = E_{inj}. \tag{13}$$

We define the mixing efficiency as

$$\eta \equiv \frac{E_p}{E_{inj}}, \tag{14}$$

which is bounded between 0 and 1. This quantity is equivalent to the cumulative mixing efficiency introduced in Peltier and Caulfield (2003), and can also be interpreted as a integrated flux Richardson number (Linden, 1979). We show in Fig. 1 how the mixing efficiency η varies with the global Richardson number

$$Ri = \frac{H\Delta b}{e_c}, \tag{15}$$

or two different initial sorted buoyancy profiles b_s, where $\Delta b = b_s(H) - b_s(-H)$.

Case (a) in Fig. 1 is the two-level configuration corresponding to a sorted profile with two homogeneous layers, for which an analytical solution exits; case (b) is the case of a initial linear sorted buoyancy profile. The kinetic energy e_c appearing in the Richardson number is not a control parameter, but one can check *a posteriori* that the total kinetic energy $E_c = V e_c$ is always of the same order of magnitude as the injected energy E_{inj}, where V is the total volume of fluid.

We see in Fig. 1 that whatever the sorted buoyancy profile, the equilibrium buoyancy profile $\overline{b}$ can be considered as almost completely homogenised in the low Richardson number limit ($Ri \ll 1$). In that case, most of the injected energy is lost in small-scale velocity fluctuations with $E_c = V e_c \simeq E_{inj}$, and the mixing efficiency is

$$\eta \simeq Ri\ \Xi[b_s] \quad \text{with } \Xi[b_s] \equiv \frac{1}{\Delta b H^2}\int_{-H}^{+H} b_s z \mathrm{d}z \ . \tag{16}$$

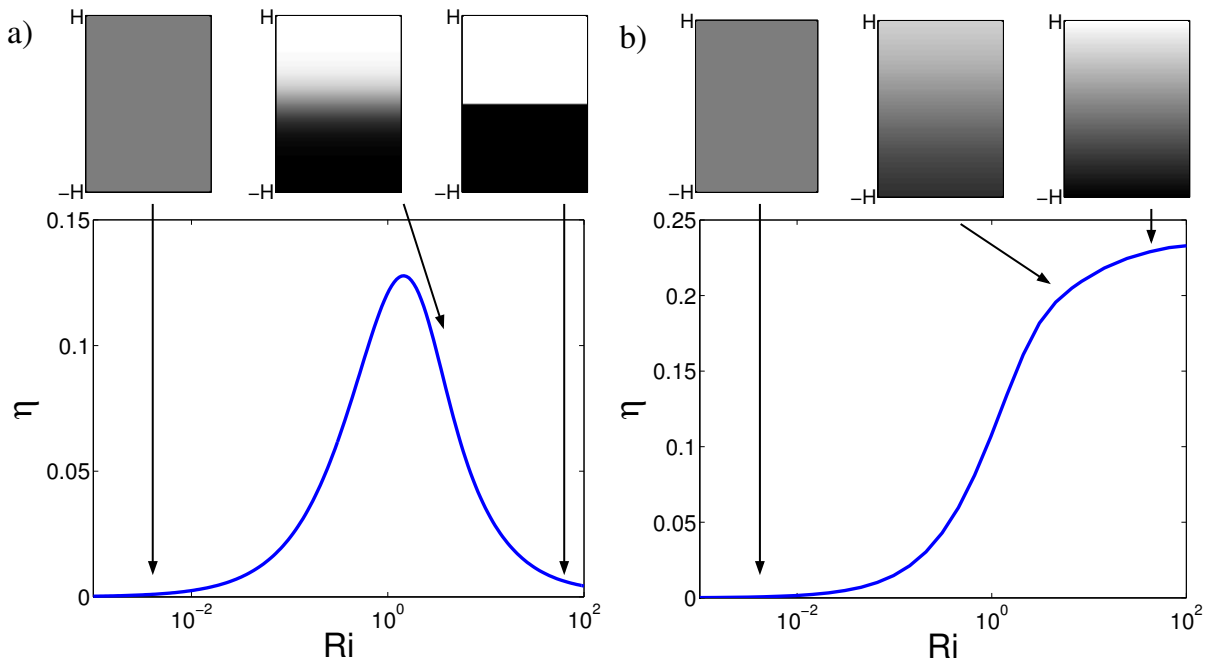

Figure 1: Variation of the mixing efficiency $\eta = E_p/E_{inj}$ with the Richardson number $Ri = H\Delta b/e_c$ a) for an initial buoyancy profile with two homogeneous layers; b) for an initial linear sorted buoyancy profile. The eddy kinetic energy e_c is homogeneous in space, with $E_{inj} = E_p + Ve_c$, where V it the volume of fluid. The three insets show the equilibrium buoyancy field $\bar{b}$ for three different values of Ri.

Thus, the mixing efficiency varies as the inverse of the Richardson number in the limit $Ri \ll 1$, with a prefactor that depends on the intitial buoyancy profile.

We see in Fig. 1 that the large Richardson behaviour of the mixing efficiency depends drastically on the initial sorted buoyancy profile b_s: the mixing efficiency decreases to zero with increasing Richardson numbers in the two-level case of Fig. 1-a, while it increases to an asymptotic value close to 0.25 in the linearly stratified case of Fig. 1-b. One can also show analytically this asymptotic value of $\eta = 0.25$ is indeed expected in a low energy limit, as a consequence of energy equipartition, provided that the stratification of the sorted profile is always strictly positive ($\partial_z b_s > 0$ for $-H \leq z \leq H$), see Venaille et al. (2016).

4 Discussion and conclusions

We have shown that several predictions for the cumulative mixing efficiency can be obtained within the framework of the equilibrium statistical mechanics theory:

1. The cumulative mixing efficiency varies as $\eta \sim 1/Ri$ in the limit of small Richardson numbers, whatever the initial buoyancy profile, which is consistent with scaling arguments given by Maffioli et al. (2016) in a forced-dissipative case.

2. The cumulative mixing efficiency tends to $\eta = 0.25$ in the limit of infinite Richardson numbers, provided that the initial buoyancy profile is sufficiently smooth. This value is a consequence of energy equipartition, and it supports previous purely kinematic arguments by McEwan (1983b,a).

3. The shape of the curve $\eta(Ri)$ depends strongly on the initial buoyancy profile, and can be non-monotonic. In the particular case of a fluid with two homogeneous layers of different buoyancy, the theory predicts a bell-shape for the cumulative mixing efficiency as a function of the bulk Richardson number with a maximum $\eta = 0.15$, just as observed experimentally in Linden (1980).

4. When the initial buoyancy profile is linear, the curve $\eta(Ri)$ is monotonic. This is consistent with previous studies on mixing in decaying experiments. In addition, the shape of the curve predicted by the equilibrium theory is consistent with empirical parameterisations for the variations of the flux Richardson number with the gradient Richardson number, see e.g. Mellor and Yamada (1982); Karimpour and Venayagamoorthy (2014); Venayagamoorthy and Koseff (2016).

To the best of our knowledge, there is so far no other theoretical results that provide such predictions in a unified framework. There remain, however, several caveats for the application of the statistical mechanics theory:

1. The ergodic hypothesis underlying the theory is a very strong assumption that may often be broken. Indeed, there are many experimental and numerical evidence showing that the efficiency of mixing often depends strongly on the energy injection mechanism, while the theory predicts that the result does not depend on how the energy is injected.

2. The theory applies to fluids in the limit of infinite Reynolds and Péclet number, while existing laboratory and numerical experiments are usually carried in intermediate regimes where mixing efficiency can be affected by finite values of molecular viscosity and diffusion, see e.g. Lozovatsky and Fernando (2013); Bouffard and Boegman (2013); Salehipour and Peltier (2015) and references therein.

3. Finally, the equilibrium theory does not predict how the system converges towards equilibrium, or what would be the energy fluxes in a forced-dissipative case. In those cases, equilibrium theory only provide a hint for the tendency of the system to be more or less efficient in mixing the buoyancy field, and other theoretical tools will be needed to model those important out-of-equilibrium features.

Despite those limitations, we believe that the statistical mechanics approach is a useful tool for the understanding of mixing in stratified turbulence, and we hope that the present work will motivate further studies in those directions.

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