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PASSIVE ADVECTION BY INHOMOGENEOUS TURBULENCE

By

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Rigorous Upper Bounds for Transport due to Passive Advection by Inhomogeneous Turbulence

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ABSTRACT

A variational procedure, due originally to Howard and explored by Busse and others for self-consistent turbulence problems, is employed to determine rigorous upper bounds for the advection of a passive scalar through an inhomogeneous turbulent slab with arbitrary generalized Reynolds number R and Kubo number K . In the basic version of the method, the steady-state energy balance is used as a constraint; the resulting bound, though rigorous, is independent of K . A pedagogical reference model (one dimension, $K = \infty$) is described in detail; the bound compares favorably with the exact solution. The direct-interaction approximation is also worked out for this model; it is somewhat more accurate than the bound, but requires considerably more labor to solve. For the basic bound, a general formalism is presented for several dimensions, finite correlation length, and reasonably general boundary conditions. Part of the general method, in which a Green's function technique is employed, applies to self-consistent as well as to passive problems, and thereby generalizes previous results in the fluid literature. The formalism is extended for the first time to include time-dependent constraints, and a bound is deduced which explicitly depends on K and has the correct physical scalings in all regimes of R and K . Two applications from the theory of turbulent plasmas are described: flux in velocity space, and test particle transport in stochastic magnetic fields. For the velocity space problem, the simplest bound reproduces Dupree's original scaling for the strong turbulence diffusion coefficient. For the case of stochastic magnetic fields, the scaling of the bounds is described for the magnetic diffusion coefficient as well as for the particle diffusion coefficient* in the so-called collisionless, fluid, and double-streaming regimes.

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1. INTRODUCTION

A quantitative theory of turbulence-induced transport is of obvious importance in many practical situations, and is also of intrinsic theoretical interest. Because of the enormous technical difficulties associated with the statistical description of nonlinear systems,¹ relatively few rigorous results are available (although our understanding of the approximation theory of such systems has grown considerably, stimulated by Kraichnan's pioneering work on the direct-interaction approximation^{2,3}). The present work is concerned with a certain class of such rigorous results. Specifically, we consider advection, by a statistically specified random velocity, of a passive scalar field through a slab with inhomogeneous boundary conditions, in the presence of (possibly weak) dissipation, but in the absence of any external sources. We will show that variational problems can be posed and practically implemented, the solutions of which provide *rigorous upper bounds* on the (conserved) mean flux of the scalar through the slab for arbitrary generalized Reynolds number R , the ratio of typical advecting velocity and dissipation parameter, and for arbitrary Kubo number K , a measure of the autocorrelation time of the velocity field.

We employ a variant and generalization of a variational method well known in the fluid mechanics literature. The history of this method began with some speculations of Malkus.⁴ He suggested that in problems of thermal convection, out of the many possible solutions of the nonlinear equations of motion, the solution which would actually be observed would be the one which *maximized the flux of heat*. This speculation turns out to be false except in certain limiting cases. However, it motivated Howard⁵ to construct a rigorous mathematical approach which, given the governing nonlinear equations, yielded an upper bound on the thermal flux. The technique, which has come to be known as the "optimum theory," was later applied with considerable success to a variety of similar problems. Busse has reviewed⁶ the progress as of 1978. All of the works described by Busse were concerned with self-consistent turbulence, in which the advected field is coupled back to the advecting flow. (In Kraichnan's terminology,⁷ the equations are *dynamically nonlinear*.) Thus, in the convection problem the velocity and the temperature fields are related *via* the Boussinesq equations, and estimates for both fields emerge simultaneously in the course of the variational calculation, which in practice can be quite involved because of the nonlinear coupling. However, it is also of interest to consider problems of *passive* advection (where the equations are *stochastically nonlinear*⁷). Such problems arise naturally in certain applications. Furthermore, the passive theory is very useful pedagogically. Most (though not all) of the features of the fully self-consistent variational principle survive in the passive version, so that one can discuss and illustrate the technique with a minimum of extraneous detail. Such a possibility was the original motivation for this work.

We shall present several versions of the theory. The so-called *basic* method, which we describe in Secs. 2-4, uses only single-time correlation functions; it thus avoids the technical difficulties, associated with two-time correlations and response, which make closures such as the direct-interaction approximation so complicated. The penalty paid for this simplicity is that the basic bound, though rigorous, is not necessarily good. For example, in the limit

of small Kubo number the basic bound does not reduce to quasilinear theory: the basic flux has a scaling different than quasilinear and the associated spatial profiles (of the mean field) are nonphysically flattened. The basic bound appears to be best and most useful in the limit of strong turbulence, exactly the regime most difficult to treat quantitatively by conventional approximation techniques. Here, the bound overestimates the true result by an amount of order unity (about 25% for an exactly solvable special case). This is not an accident. Unlike existence-type proofs such as that of the KAM theorem, which are often only able to provide estimates for critical parameters many orders of magnitude different than the physical ones, the present constructive technique exploits important physical balances in such a way that the bounding estimate is guaranteed to be "reasonable." (Admittedly, the definition of "reasonable" is somewhat subjective.)

Even if the basic bound were never good, it would still be of interest, as the balance from which it is derived must continue to hold even when more details of the governing equations are considered. However, it is useful to determine a bound which scales correctly in all regimes of R and K , and we are able to accomplish this in Sec. 5 by extending the method to include *two-time constraints*. We believe this is the first application of two-time constraints in the context of the optimum theory.

1.1 Motivation

The motivation for our work on turbulent transport is our interest^{8,9} in the transport of heat in magnetically confined plasmas, although we shall not discuss that problem here in detail. (For some general remarks, see Sec. 7.) For example, the slab in question might be an idealization of the edge region of a tokamak. Of course, the turbulence in such a region is generally self-consistent. However, because even very approximate model equations for self-consistent plasma fluctuations tend to be quite involved, we consider it useful to study first, and in its own right, the simpler passive problem. Furthermore, there does exist an important class of truly passive problems, involving the collision-induced transport across a KAM surface bounding a region of stochasticity, where the dynamics are Hamiltonian in the absence of collisions. This class includes several examples of practical interest. Two applications from plasma physics are (1) Dupree's original discussion of the velocity space diffusion coefficient in the limit of strong turbulence,¹⁰ and (2) test particle transport across a region of given stochastic magnetic fields bounded by global magnetic flux surfaces. (See various references cited in Ref. 8.) Both of these examples are briefly discussed further below and in Sec. 6, although our principal concern in this paper is with the general formalism.

Ultimately, one would like to obtain a usable and believable theory of plasma turbulence. However, it has been clear for some time that the class of practical problems which arises in the theory of magnetically confined plasmas presents severe difficulties for statistical turbulence theories. These plasmas are both *anisotropic* and *inhomogeneous*. All three spatial dimensions are physically distinct, and at least one velocity space variable may be

required as well. The resulting plethora of variables leads to a computational challenge of enormous complexity¹¹ when closures such as the direct-interaction approximation are considered, even with the aid of modern supercomputers.

Therefore, other approximation procedures have been advocated, beginning with Dupree's resonance-broadening theory.¹⁰ More recently, in addition to the by now relatively well-known simpler cousins of the direct-interaction approximation,¹² which unfortunately have not been much used for plasma problems (although see Ref. 13), the so-called "clump" algorithm¹⁴ has been advanced as a closure technique useful for a variety of plasma and fluid turbulence problems,¹⁵ and its predictions have been pursued to the point of computing numerical coefficients.^{16,17} However, that theory invokes many approximations of dubious quantitative validity, and its application to the dynamically interesting fluctuations which dominate transport has been questioned on conceptual grounds as well.¹⁸ A sounder procedure seems highly desirable.

It has been argued¹⁹ that problems of plasma turbulence may be simpler than the typical problem of incompressible neutral fluid turbulence because wave-like motions in the plasma lead to order unity balances between linear and nonlinear terms in the final saturated state, whereas the Reynolds number of the fluid is typically very large. Such arguments should not be carried too far, since waves are not described by the Reynolds number but by other dimensionless parameters. It is true that relatively simple arguments (of the mixing length variety) succeed in estimating the rms fluctuation level in many plasma turbulence problems.²⁰ However, determination of the associated transport is more delicate. Quasilinear calculations are sometimes successful. However, it is possible to exhibit systems which saturate at finite fluctuation levels but whose transport vanishes identically.²¹ Plasma systems often saturate at the border between weak and strong turbulence. Particle simulations sometimes demonstrate considerable sensitivity of transport to dissipation parameters.²² Formally, while transport is fully determined if the fluctuation spectra of all variables are known, including the cross-correlations between variables, those cross-correlations (phase differences) are extremely difficult to determine precisely by purely analytic methods. Dimensional considerations are quite useful,²³ but cannot determine numerical coefficients or scaling with various dimensionless parameters.

The severe difficulties of a primarily analytic approach to practical turbulence problems lead one to search for a hybrid analytical/computational method. An analogy may be useful. For linear theory, such an approach has been very successfully developed in the study of the magnetohydrodynamics (MHD) of magnetized plasmas, in the form of the energy principle δW of Bernstein *et al.*²⁴ That principle has led to important physical insights with regard to the balances necessary for linear stability, and has suggested computational techniques superior in some cases to those which would be suggested by straightforward numerical analysis of the original dynamical equations. The method which we begin to explore here is similar in some general ways to the energy principle. Both methods are variational. In both, there is a functional which describes the energy balance of the system.

Variations of both functionals lead to Euler-Lagrange equations (henceforth called the Euler equations for brevity), the spectral properties of which describe important macroscopic features of the system. However, there are profound differences, both philosophical and technical, between the methods as well, and the present work should not be thought of as a generalization of δW . In the MHD applications the Euler equations are linear and dissipation-free, and their eigenvalue spectrum is related to linear stability. There is no element of statistical behavior in δW . In the present case the formalism applies to turbulence. The Euler equations are nonlinear (for the self-consistent case; they are linear for the passive problems described in this paper) and dissipative, and their spectral behavior describes bounds on the transport of macroscopic quantities such as particles or heat in a fully nonlinear, statistically steady state.

1.2 General approach

Although the basic approach for self-consistent problems is thoroughly described by Busse,⁶ it is useful, before beginning the detailed calculations, to describe it in general terms and to comment on its salient features. We consider the random, passive advection of a scalar field $T(\mathbf{x}, t)$. (The notation is chosen because of our interest in the fusion application to thermal transport. However, T need not necessarily be temperature; we shall refer to it neutrally as "concentration.") Although generalizations are possible, we shall assume that T is described by

$$\frac{\partial}{\partial t} T(\mathbf{x}, t) + \nabla \cdot [\mathbf{u}(\mathbf{x}, t) T] + \mathcal{L}T = 0, \quad (1.1)$$

where $\mathbf{u}$ is a stationary Gaussian random variable independent of T , $\mathcal{L}$ is a dissipative linear operator in conservation form (such as $-\kappa \nabla^2$), and we work in a (for now, unspecified) bounded region with prescribed boundary conditions, inhomogeneous in the x direction, periodic in the others. Usually, we also assume that $\mathbf{u}$ is statistically homogeneous. The simplest boundary conditions specify the field rigidly (no fluctuations) at the boundaries $x = 0$ and $x = L$. (See Sec. 7 for a discussion of the relevance of this assumption to practical problems, and of the relationship of L to the dimensions of a confinement vessel like the tokamak.) A two-dimensional slab situation is sketched in Fig. 1. Because Eq. (1.1) is linear, only the concentration difference $\Delta T \doteq T(L) - T(0)$ is relevant. Because Eq. (1.1) is in conservation form and because no external sources are allowed, the total flux Γ_{tot} (including a classical contribution Γ_{cl} from $\mathcal{L}$ as well as the advective or "anomalous" part $\Gamma \doteq \bar{\mathbf{x}} \cdot \langle \delta \mathbf{u} \delta T \rangle$) is conserved. Here $\delta T \doteq T - \langle T \rangle$ and $\langle \dots \rangle$ denotes the ensemble average (see Sec. 1.4 below) over the statistics of the advecting velocity field. The mean concentration profile, although pinned at the walls, is free to adjust itself in the interior and must be determined self-consistently. In Fig. 1 the heavy solid line shows a typical profile $\langle T \rangle(x)$ for the boundary conditions $T(0) = -\Delta T > 0$, $T(L) = 0$, in a moderately turbulent situation. Also shown are typical profiles of the constituents $\Gamma_{\text{cl}}(x)$ and $\Gamma(x)$ of the total conserved flux, normalized to Γ_{tot} . It is important to note that, with the assumed boundary conditions, $\Gamma(x)$ vanishes at the boundaries, so the flux through the

wall is carried by entirely classical processes. (The profiles shown are the actual results from the reference model of Sec. 2 with $R = 5$, $K = \infty$, although this detail is not important for this introductory discussion.)

Consider a one-dimensional slab situation, and assume for simplicity that the advecting field is independent of space: $u = u(t)$. The problem then contains just two fundamental dimensionless parameters, the generalized Reynolds number²⁵ R and the Kubo number²⁶ K . To define these, note the following. The velocity fluctuations, being Gaussian, are described by exactly two parameters—their rms size $\bar{u}$, and their autocorrelation time τ_{ac} . (If we introduce the time correlation function

$$U(\tau) \doteq \langle \delta u(t' + \tau) \delta u(t') \rangle,$$

we have

$$\bar{u}^2 = U(0)$$

and

$$\tau_{ac} \doteq \left[\int_0^\infty d\bar{\tau} U(\bar{\tau}) \right] [U(0)]^{-1}.$$

An equivalent autocorrelation time involving the spatial correlation length can often be defined when u depends on space as well.²⁷ We shall describe the classical dissipation by a diffusivity κ . It is natural to normalize T to $|\langle \Delta T \rangle|$, lengths to L , velocities to $\bar{u}$, and, thus, times to

$$\tau_L \doteq L/\bar{u},$$

which is a macroscopic “eddy” or “circulation” time. Define also a hydrodynamic time τ_h by

$$\tau_h \doteq L^2/\kappa, \quad (1.2)$$

the time for a perturbation to diffuse across the slab by classical processes. Then, we may define the generalized Reynolds number R by

$$R \doteq \tau_h/\tau_L = \bar{u}L/\kappa, \quad (1.3)$$

and define the Kubo number K by

$$K \doteq \tau_{ac}/\tau_L = \bar{u}\tau_{ac}/L. \quad (1.4)$$

The Reynolds number is just the hydrodynamic time in our dimensionless units, while the Kubo number is the dimensionless autocorrelation time. [The nomenclature “(generalized) Reynolds number” is intended to invoke the general interpretation of R as a ratio of eddy to

classical diffusivity, and not the more specific usage related to dissipation of momentum.] For future use, note that

$$K/R = \tau_{ac}/\tau_h. \quad (1.5)$$

Although the total flux Γ_{tot} is conserved, its constituents Γ_{cl} and Γ separately depend on x :

$$\Gamma_{tot} = \Gamma_{cl}(x) + \Gamma(x).$$

However, as we will show, a barring operation in space can be defined (in simple cases, it is just $\int_0^1 dx$) such that

$$\Gamma_{tot} = \bar{\Gamma}_{cl} + \bar{\Gamma},$$

where $\bar{\Gamma}_{cl}$ is completely known in terms of R and the boundary conditions. (In the simplest case $\bar{\Gamma}_{cl} = -\kappa/L \sim R^{-1}$.) Thus, attention shifts to the nonlinear quantity $\bar{\Gamma}$, an appropriate spatial and ensemble average of the advective contribution to the total flux. Conventional closure approximations (see many references cited in Ref. 3) attempt to predict $\bar{\Gamma}$ as accurately as possible by determining approximate forms for various triplet correlation functions. The philosophy of the optimum theory⁵ is different. Here, one sets the more tractable goal of determining merely an *upper bound* $\gamma(R, K)$ on $\bar{\Gamma}$. To do this, one considers an enlarged manifold of fields which includes not only the actual solutions of the equations of motion but also other, nonphysical fields which, however, share certain important balance constraints with the physical solutions. It is easier to work in the larger space, and it turns out that one gains thereby the power of variational methods, whereas the physical solutions cannot, in general, be derived from a variational principle.

The choice of constraints is to some extent arbitrary. (To date, at least, the notion of a "best" constraint has not been formalized.) Capitalizing on the experience of previous workers, the basic procedure we study here is to consider the balance equation for the steady-state (generalized) fluctuation energy $\langle \delta T^2(x, t) \rangle / 2$. (A both more neutral and more correct nomenclature would be to call $\langle \delta T^2 \rangle$ the "scalar variance," since, depending on the interpretation of T , the variance may, for example, be more closely related to entropy than to energy. However, since we will not need to make such distinctions in this paper, we prefer the phrase "fluctuation energy," as it invokes a more specific and physical interpretation.) The balance equation has the general form²⁸

$$\mathcal{P}(x) = \mathcal{T}(x) + \mathcal{D}(x),$$

where $\mathcal{P}$ stands for "production," $\mathcal{T}$ stands for "transfer," and $\mathcal{D}$ stands for "dissipation." The transfer term is the troublesome one; it is the divergence of the triplet correlation between the advecting flow and δT^2 , and thus (by definition) suffers from the closure problem. However, because of the conservation properties of the equations, the offending triplet term can be *annihilated* by an appropriate integration across the layer. The resulting, spatially averaged equation,

$$\bar{\mathcal{P}} = \bar{\mathcal{D}},$$

describes the global balance between production and dissipation. It also involves, through the production term, the unknown, self-consistent gradient of the mean scalar; that, however, can be eliminated in favor of fluctuation-related quantities by an integration of the mean continuity equation. (That integration defines the barring operation.) The result is a nonlinear constraint on the flux, and the basic variational problem is to maximize the flux subject to that constraint. Note that because this basic bound uses only equal-time correlations, it does not involve the Kubo number and essentially assumes $K = \infty$. We shall thus call the basic bound $\gamma_\infty(R)$.

It is important to stress that although the velocity fluctuations are not self-consistent, the mean concentration gradient is self-consistently determined as a functional of the boundary conditions and imposed fluctuations. This is the opposite of the model often adopted in problems of plasma transport, in which the mean gradient is assumed to be a fixed, specified function (often a constant), presumably supported by external sources. In this extreme case the variational principle predicts in the limit of large R an unphysically large result. Worse, for fixed gradients the extension of the principle to self-consistent problems is ill-posed and predicts an upper bound of infinity. The self-consistent relaxation of the profile appears to be an important physical process. We discuss this issue further in Sec. 7.

In the most straightforward mathematical implementation of the basic bound, the energy balance constraint is included by means of a Lagrange multiplier. Particularly in the self-consistent problems, but true in the passive case as well, the mathematics for this approach becomes slightly awkward because of the need to determine the multiplier. (For some self-consistent problems, two multipliers are required.) However, Howard has shown⁵ that an equivalent minimum principle can be formulated in which the fundamental Lagrange multipliers are not necessary. (More precisely, they are present, but vanish.) It is the minimum principle which we use here.

Additional constraints can be added to refine the bound. Quantitative refinement of the basic bound would follow by consideration of additional equal-time balances, and such calculations have been performed for self-consistent cases.²⁹ However, qualitative improvement to take account of a finite Kubo number requires a nontrivial extension of the formalism to include two-time constraints. These are added by means of a time-dependent Lagrange multiplier, the use of which in the context of the optimum theory appears to be new here.

1.3 Scaling laws

We shall now describe the true ("physical") scalings which would follow from a complete solution of the passive advection problem, and then state the scalings of the bounds we will obtain later. In presenting these results, we shall maintain in this section a distinction between dimensional fluxes $\bar{\Gamma}$ and their dimensionless values, which we shall call γ .

Furthermore, it is often fruitful to introduce the notion of an “anomalous diffusivity” D_a , the (spatially constant) coefficient in the expression

$$\bar{\Gamma} = -D_a \langle \Delta T \rangle / L = D_a |\langle \Delta T \rangle| / L;$$

in terms of the dimensionless flux γ , one has

$$D_a = \bar{u} L \gamma. \quad (1.6)$$

The dimensions of D_a are [length]²/[time], and it is useful to think of D_a in terms of the random walk scaling

$$D_a \sim \Delta x^2 / \Delta t \sim \Delta v^2 \Delta t, \quad (1.7)$$

for various choices of fundamental step sizes and step times. However, that we define a diffusivity does *not* necessarily mean that the transport is local in space. When the fluctuations are strong, macroscopic correlations arise, the effects of the boundary conditions are felt throughout the entire domain, the mean concentration profile is flattened, and boundary layers emerge. Nevertheless, D_a is a useful measure of the size of the transport.

To describe the true physics picture, we begin with the classical flux, which serves as a reference: $\gamma_{cl} = \kappa / \bar{u} L$, or

$$\gamma_{cl} = R^{-1}. \quad (1.8)$$

Of course, this flux is caused by microscopic effects not explicitly described by the equation of motion (1.1).

In addition to γ_{cl} , there are three distinct advective fluxes, resulting from different sets of fundamental steps and times. Two of these are varieties of the “quasilinear” scaling $D_Q \sim \Delta v^2 \Delta t$, where $\Delta v \sim \bar{u}$ and Δt is taken to be a time characteristic of the unperturbed motion: $\Delta t = \min(\tau_{ac}, \tau_h)$. For $\tau_{ac} \ll \tau_h$ ($K \ll R$) and $\tau_{ac} \ll \tau_L$ ($K \ll 1$), we find the usual quasilinear result (details are presented in Sec. 5.1)

$$D_q \sim \bar{u}^2 \tau_{ac},$$

or in dimensionless units, recalling Eqs. (1.4) and (1.6),

$$\gamma_q \sim K \quad (K \ll R, K \ll 1). \quad (1.9)$$

For $\tau_h \ll \tau_{ac}$ ($K \gg R$) and $\tau_h \ll \tau_L$ ($R \ll 1$), we obtain what we shall call the “hydrodynamic” quasilinear diffusion coefficient

$$D_h \sim \bar{u}^2 \tau_h$$

or, using Eqs. (1.2), (1.3), and (1.6),

$$\gamma_h \sim R \quad (R \ll K, R \ll 1). \quad (1.10)$$

These results are valid for K or R sufficiently small, as indicated. For R sufficiently small, the classical (laminar) contribution dominates the advective ones, as one can see as follows. The classical flux will dominate the hydrodynamic one when [using Eqs. (1.10) and (1.8)]

$$1 > \frac{\gamma_h}{\gamma_{cl}} \sim K^2.$$

Similarly, from Eq. (1.9), the classical flux will dominate the quasilinear one when

$$1 > \frac{\gamma_q}{\gamma_{cl}} \sim KR.$$

For $K \gg 1$ and $R \gg 1$, the correct scaling is that of strong turbulence: $D_s \sim \Delta x^2 / \Delta t$, where $\Delta x \sim L$, the width of the layer, and $\Delta t \sim \tau_L$, the time to cross the layer. Thus

$$D_s \sim L^2 / \tau_L \sim \bar{u} L,$$

or

$$\gamma_s \sim 1 \quad (R \gg 1, K \gg 1). \quad (1.11)$$

It is important to note that although the result (1.11) does not involve the classical diffusivity κ explicitly, the classical processes are important nevertheless: In their absence, steady states could not be achieved and the boundary conditions could not be met. [κ multiplies the highest derivative in Eq. (1.1), so the problem in the limit $\kappa \rightarrow 0$ ($R \rightarrow \infty$) is one of singular perturbations.]

In fluid dynamics, the scaling (1.11) is the familiar result for the eddy diffusivity of test fluid elements in strongly turbulent flows.²⁸ There are similar fluid-like results in plasma physics—see, for example, the nonlinear theory of convective cells.^{30,3} Furthermore, this result is very reminiscent of Dupree's original expression for the velocity space diffusion coefficient in the limit of strong turbulence.¹⁰ The interpretation of that result has always been somewhat unclear, as Dupree's work was done in the dissipation-free, Vlasov limit, in which case particles must remain confined to the stochastic region and the global flux into the nonstochastic region must vanish. A vanishingly small amount of collisions leads to a quite finite flux, however, and it is remarkable that a rigorous, reasonable bound can be given for the magnitude of that flux. The formulation of a principle for that situation is described briefly in Sec. 6.1.

A similar situation can be found in the theory of plasma transport in the presence of stochastic magnetic fields.⁸ If we consider a region of static, stochastic magnetic fields, bounded on both sides by good KAM surfaces, collisional effects are necessary in order to permit a finite amount of flux across the region. We discuss this situation further in Sec. 6.2.

In passing, we note that the preceding formulas for the diffusion coefficients may be used to provide alternative interpretations of R and K as ratios of diffusivities. Equation (1.3) can be written as

$$R \sim D_s/\kappa,$$

Eq. (1.4) becomes

$$K \sim D_q/D_s,$$

and Eq. (1.5) becomes

$$K/R \sim D_q/D_h.$$

The true scaling situation is summarized in Fig. 2, which identifies the various regimes in the two-parameter space of K and R . The numbering of the regimes is arbitrary. For R sufficiently small (to the left of line AXC), classical transport dominates, giving rise to smooth, nearly constant gradients; we call this regime "laminar conduction." In the opposite limit, the nonlinear flux dominates; we call this regime "turbulent advection." Characteristic of this regime is the existence of boundary layers, which must form in order to reconcile conservation of total flux with the fact that the advective flux vanishes at the boundaries. We shall call the regime $R < K$ the "hydrodynamic" regime and label it by "h"; in this regime the autocorrelation time is essentially irrelevant. We shall call the opposite limit $K < R$, in which τ_{ac} is important, the "kinetic" regime and label it by "k." This nomenclature is intended to be reminiscent of various kinetic (*i.e.*, velocity space) processes which can be physically responsible for a short autocorrelation time.

Upon collecting the results of the various random walk arguments, we have, in dimensionless units, the classical flux, which serves as a reference,

$$\gamma_{cl} = R^{-1}, \quad (1.12a)$$

and the various nonlinear fluxes,

$$\gamma_q \sim K, \quad (1.12b)$$

$$\gamma_h \sim R, \quad (1.12c)$$

$$\gamma_s \sim 1. \quad (1.12d)$$

For purposes of the following discussion, we shall ignore the numerical coefficients implicit in Eqs. (1.12) and treat these scaling relations as equalities. As we have stated, the classical flux dominates the hydrodynamic flux when $\gamma_h/\gamma_{cl} = R^2 < 1$, or when $R < 1$. The classical flux dominates the quasilinear flux when $\gamma_q/\gamma_{cl} < 1$, or when $KR < 1$; this inequality divides the kinetic quasilinear regime 2k into two subregimes. Thus,

classical flux dominates in regimes 1k, 2k(a), 1h, and 2h, the quasilinear flux dominates in regime 2k(b), and strong turbulence dominates in regimes 3k and 3h. The solid lines in Fig. 2 identify transitions between different functional forms for the advective flux. There are no discontinuities in scaling, for either the advective or the total flux, across any boundary in the parameter space. For example, one can move from regime 2k to 3k by increasing K at constant R from $K < 1$ to $K > 1$. At the transition $K = 1$, one has

$$\gamma_q(K=1) = \gamma_s(K=1) = 1.$$

Similarly, at the transition between regimes 1k and 1h one has

$$\gamma_q(K=R) = \gamma_h(K=R) = K = R.$$

As yet another example, consider the total flux as one moves from regime 2h to 3h. Classical flux dominates the hydrodynamic flux in regime 2h, while strong turbulence dominates in regime 3h. At the transition $R = 1$, all three fluxes become equal:

$$\gamma_{cl}(R=1) = \gamma_h(R=1) = \gamma_s(R=1) = 1;$$

as one moves to $R > 1$, the classical flux decreases as R^{-1} while the strong turbulence formula $\gamma_s = 1$ replaces the hydrodynamic formula $\gamma_h = R$.

This summarizes the true scaling picture for arbitrary R and K . We now turn to the predictions of the bounding theory. As we have stated, the simplest prediction is obtained by considering only equal-time constraints, from which the Kubo number cannot emerge. Thus, the bound $\gamma(R, K)$ becomes just $\gamma_\infty(R)$, and it is clear that the basic bound cannot always be good, as the formalism cannot discriminate between the “quasilinear” limit of short autocorrelation time (K small) and the “strong turbulence” limit of large autocorrelation time (K large). Indeed, the scaling for the basic bound can be stated very simply: it predicts fluxes which *scale like the fluxes in the hydrodynamic regime*. By their rigorous construction, these bounds, although independent of K , remain valid for all K . This is also clear heuristically, because according to Fig. 2 and Eqs. (1.12) the fluxes decrease as one moves vertically downward (R constant) from the hydrodynamic regime into the kinetic regime.

Actually, the failure of the basic bound to recognize τ_{ac} or finite K is not as troublesome as one might expect initially. First, quasilinear expressions can be computed straightforwardly from first principles, independently of considerations of bounds. (We review the analytic quasilinear theory in Sec. 5.1.) Second, in practice turbulent systems driven by mean gradients (e.g., shear flows in fluids or drift waves in plasmas) often saturate at the boundary between weak and strong turbulence, when $D_s \sim D_q$, or when $K \sim 1$. Thus, the strong turbulence bound is of considerable practical interest. Nevertheless, it is conceptually desirable and useful for quantitative accuracy to develop a version of the theory which is capable of discriminating between large and small K . We show how to

do this in Sec. 5 by introducing two-time constraints. The qualitative behavior of the improved bound can be described by the interpolation formula

$$\gamma^{-1}(R, K) = \gamma_{\infty}^{-1}(R) + \gamma_q^{-1}(K). \quad (1.13)$$

This result is literally true only for an exactly soluble special case which we describe in Sec. 5. However, its qualitative validity is much more general. Clearly $\gamma \rightarrow \gamma_q = K$ when K is sufficiently small, whereas the basic bound γ_{∞} is recovered as $K \rightarrow \infty$. Equation (1.13) is analyzed more thoroughly in Sec. 5, where we show that it yields the physical scalings in all regimes of R and K .

1.4 Notation for averages

To conclude this introduction, we must discuss certain notation. Several kinds of averages will be employed in this work. The most fundamental one is the statistical or ensemble average over the specified distribution of the advecting field and, possibly, any random initial conditions. We shall denote the ensemble average by $\langle \dots \rangle$. We assume that the system is statistically temporally stationary, and is spatially homogeneous in all but the single direction x in which the inhomogeneous boundary conditions are applied. Thus,

$$\langle A(\mathbf{x}, t) \rangle = \langle A \rangle(\mathbf{x}).$$

When the advecting field is a random number u whose probability density function is $P(u)$ (see Sec. 2), one has

$$\langle A \rangle(\mathbf{x}) \doteq \int_{-\infty}^{\infty} du P(u) A(\mathbf{x}; u). \quad (1.14a)$$

More generally, a functional integral³¹ is indicated:

$$\langle A \rangle(\mathbf{x}) \doteq \int D[u] P\{u\} A(\mathbf{x}; \{u\}). \quad (1.14b)$$

(The braces indicate functional dependence. $D[u]$ stands for the volume element in function space.)

A second average, $\bar{A}$, related to (but not necessarily equal to; see Sec. 3.2) spatial averaging in the inhomogeneity direction x , will also emerge in the course of solving the continuity equation as a boundary value problem to eliminate the mean scalar field in favor of two-point correlations. Unfortunately, this usage of angular brackets and bars is the opposite of the convention which has been adopted in the fluid literature on the optimum theory.⁶ Our choice of notation was adopted neither arbitrarily nor without some considerable reluctance. However, we feel our convention is more physically suggestive than the original. In closure theory,^{1,3} the notation $\langle A \rangle$ is strongly preferred for the

ensemble average, which is the fundamental ingredient here. (In the original applications, the preferred status of the ensemble average was blurred, as it was also realized by a spatial integral, but over the homogeneous directions only.⁶) We feel our notation is more in accord with standard practice in the theory of stochastic differential equations,³² as well as with the usages in the plasma physics literature. There, in addition to ensemble averages, a barring operation is frequently introduced in perturbation theory to determine solubility constraints by annihilating unwanted terms. An annihilation procedure is central to the variational method as well. Furthermore, when we introduce time-dependent constraints, it becomes natural to augment the x integration by time integration; the use of the bar notation for time averaging is in agreement with the convention in ergodic theory.

1.5 Organization

The remainder of the paper is organized as follows. We treat most thoroughly, in Secs. 2 through 4, the case of the single equal-time energy-balance constraint, the result of which we call the basic bound $\gamma_\infty(R)$. Because of its pedagogical importance, we devote Sec. 2 to a detailed discussion of the arguably simplest model to which the method can be applied: transport of a passive scalar, through a one-dimensional slab with inhomogeneous boundary conditions, by a velocity field spatially and temporally constant in each realization of a Gaussian ensemble (the limit of infinite Kubo number). For this problem, which we call the reference model, both the exact solution and the bound can be found analytically, and can be compared (favorably).

In Sec. 3 we generalize the calculation of the basic bound to include several dimensions, arbitrary space and time dependence of the advecting field, and general boundary conditions. The Euler equations for the passive scalar lead to an integral equation, for the advective flux as a function of space, from whose solution the bounding curve relating the total flux through the system to the Reynolds number can be obtained. This integral equation is one of the principal results of the paper. It is quite general, as it is couched in terms of Green's function for the (unspecified) dissipative linear operator in the dynamical equation of motion, with the associated boundary conditions. The emphasis on Green's technique is a feature of the present work. There are really two uses of Green's function, concerning (1) the treatment of the mean continuity equation, and (2) the derivation of the integral equation for the bounding advective flux. First, previous workers used mostly very simple dissipative operators, such as $-d^2/dx^2$, and specific, simple boundary conditions, and constructed their variational principles by explicit integration of the continuity equation. Because such results have the operator and boundary conditions built in, the resulting principles are not readily generalizable. When the results are instead couched in terms of Green's function for the mean field, the structure of the theory becomes much clearer. Second, while in the self-consistent cases coupled, nonlinear Euler equations emerge, in the present passive case there is one, linear Euler equation, which is also amenable to solution *via* Green's function, this time for the fluctuations.

In Sec. 4 we return to the reference model, and derive and numerically solve the direct-interaction approximation for that model. This calculation is not logically related to the bounding theory, but it enables one to contrast in a simple yet nontrivial situation the optimum theory with more conventional closures. Furthermore, the direct-interaction approximation is not usually studied in inhomogeneous situations, and is interesting in its own right.

In Sec. 5 we generalize the basic formalism to allow for two-time constraints. We solve the variational problem for the generalized (finite K) reference model explicitly for one simple constraint, and are able to derive a bound which has the correct (physical) scalings in all regimes of R and K . Although much work remains to be done on the two-time theory, it is clear that the method we introduce is more general than the specific application we study here.

The previously mentioned plasma physics applications are discussed in Sec. 6. We devote Sec. 7 to discussion and conclusions. Several appendices are included: (A) remarks on the meaning of the functional derivative used in deriving the Euler equations; (B) discussion of the use of Lagrange multipliers in forming the variational principles; (C) derivation of the direct-interaction approximation for the passive flux; (D) a sketch of the numerical procedure used to solve the direct-interaction approximation; and (E) a brief discussion of the limit $\tau_{ac} \rightarrow 0$, which is somewhat pathological.

With this introduction, we shall now begin our detailed calculations by considering a special case which can be solved exactly.

2. PEDAGOGICAL EXAMPLE: ONE DIMENSION, INFINITE KUBO NUMBER

The purposes of this section are two-fold. First, we wish to give a pedagogical introduction to the variational method, which has not been applied to passive problems and, at least viewed from the discipline of plasma physics, is not well known. Second, we wish to work out a simple reference case in great detail, so that the general formalism in the next section can be checked against, and compared to, a known limit. The model we choose is a variant of the stochastic oscillator of Kubo²⁶ and Kraichnan.⁷ Kraichnan and others³ have turned repeatedly to the basic stochastic oscillator in order to motivate and illustrate various features of closure theory; we hope that the results described here will be of similar utility.

2.1 The reference model

As a pedagogical model, let us consider a specific, one-dimensional version of Eq. (1.1):

$$\frac{\partial}{\partial t} T(x, t) + u \frac{\partial T}{\partial x} - \kappa \frac{\partial^2 T}{\partial x^2} = 0,$$

together with

$$\begin{aligned} T(0, t) &= T_0(t), \\ T(L, t) &= 0. \end{aligned}$$

Here u is a Gaussian random number, independent of x and t , with mean zero and with standard deviation $\bar{u}$:

$$\bar{u} \doteq \langle \delta u^2 \rangle^{1/2}.$$

At this point, the specified boundary function T_0 may also be random. The boundary conditions we have chosen are not the most general ones possible, but are adequate for the purposes of this introductory discussion. In general, one must also specify an initial condition $T(x, 0)$. However, we shall consider only time-asymptotic, statistically steady states, which do not depend on $T(x, 0)$.

As in the Introduction, we introduce a generalized Reynolds number R , defined by Eq. (1.3). Except for possible parameters describing the random boundary condition, R is the unique dimensionless parameter. (The Kubo number K is ∞ . This limit provides a particularly severe test of any statistical theory.⁷) Upon normalizing T to $\langle T_0 \rangle$, x to L , u to $\bar{u}$, and t to $\tau_L \doteq L/\bar{u}$, we can write

$$\frac{\partial}{\partial t} T(x, t) + u \frac{\partial T}{\partial x} - R^{-1} \frac{\partial^2 T}{\partial x^2} = 0, \quad (2.1)$$

together with

$$\begin{aligned} T(0) &= 1 + \delta T_0(t), \\ T(1) &= 0. \end{aligned}$$

Since we have assumed that u is time-independent, asymptotic time dependence of T arises only from fluctuations in the boundary condition, $\delta T_0(t)$. If δT_0 does not depend on time (although it may still be random), then asymptotically $T = T(x)$. In the simplest case, $\delta T_0 \equiv 0$, and we arrive at our *reference model*:

$$u \frac{d}{dx} T(x) - R^{-1} \frac{d^2 T}{dx^2} = 0, \quad (2.2a)$$

with

$$\begin{aligned} T(0) &= 1, \\ T(1) &= 0. \end{aligned} \quad (2.2b)$$

Note that these boundary conditions are equivalent to

$$\begin{aligned} \langle T \rangle(0) &= 1, & \delta T(0) &= 0, \\ \langle T \rangle(1) &= 0, & \delta T(1) &= 0. \end{aligned} \quad (2.3)$$

Since the fluctuations vanish at the boundary, we call these boundary conditions *rigid*. We shall return in Sec. 3 to the case where $\delta T_0 \neq 0$.

2.2 Exact solution of the reference model

The exact solution of Eqs. (2.2) is

$$T(x) = \exp(\tfrac{1}{2}Ru x) \frac{\sinh(\tfrac{1}{2}Ru(1-x))}{\sinh(\tfrac{1}{2}Ru)}. \quad (2.4)$$

As $R \rightarrow 0$, $T(x) \rightarrow 1 - x$, the profile of laminar conduction. As $R \rightarrow \infty$, boundary layer effects ensue: for $u > 0$, $T \sim 1$ for $x \neq 1$; for $u < 0$, $T \sim \exp(-R|u|x)$ for $x \neq 1$. Representative realizations are shown in Fig. 3.

We shall now proceed to compute various mean quantities. As we discussed in the Introduction, one must distinguish between two kinds of averages. For any random variable $A(x; u)$, we shall denote the statistical or ensemble average by Eq. (1.14a), where in dimensionless units

$$P(u) = (2\pi)^{-1/2} \exp(-u^2/2). \quad (2.5)$$

We will also need a barring operation, the role of which here is to perform a spatial average over the layer:

$$\bar{A} \doteq \int_0^1 d\bar{x} \langle A \rangle(\bar{x}).$$

The mean scalar field follows immediately by ensemble-averaging Eq. (2.4). In performing that operation, it is convenient to employ a symmetrization in u to replace $\exp(\tfrac{1}{2}Ru x)$ by $\cosh(\tfrac{1}{2}Ru x)$, then to use a hyperbolic identity. One obtains

$$\langle T \rangle(x) = \frac{1}{2} \left(1 - \left\langle \frac{\sinh(Ru(x - \tfrac{1}{2}))}{\sinh(\tfrac{1}{2}Ru)} \right\rangle \right), \quad (2.6)$$

the second term representing the deviation from the spatial mean $\bar{T} = 1/2$. It does not appear possible to express the ensemble average in Eq. (2.6) in a useful closed form. However, the integral over the Gaussian distribution (2.5) can be performed by standard

techniques of numerical integration. Representative concentration profiles are displayed in Fig. 4. Note that for a Reynolds number smaller than about 5, the profiles are quite similar to the purely laminar one ($R = 0$). For these Reynolds numbers, the classical flux dominates the advective flux, as we shall discuss in the next several paragraphs.

We now turn to the flux. (In this and the following sections, since we work exclusively in dimensionless units we shall return to the notation Γ for the true flux, reserving γ for the bound in the variational theory.) The advective flux Γ is defined by

$$\Gamma(x) \doteq \langle \delta u \delta T(x) \rangle = \langle u T(x) \rangle, \quad (2.7)$$

one has

$$\Gamma(0) = \Gamma(1) = 0 \quad (2.8)$$

because of the boundary conditions (2.3) on δT . A general relation, which will be of considerable use in later sections as well, follows from the statistical mean of Eq. (2.2a) and expresses conservation of the total flux Γ_{tot} :

$$\frac{d}{dx} \Gamma(x) - R^{-1} \frac{d^2}{dx^2} \langle T \rangle(x) = 0. \quad (2.9)$$

This is the mean continuity equation. (It remains true when u depends on time, under the assumption of statistical stationarity.) Upon integrating Eq. (2.9), we find

$$\Gamma_{\text{tot}} \doteq -R^{-1} \frac{d}{dx} \langle T \rangle(x) + \Gamma(x) = \text{const.} \quad (2.10a)$$

$$= \bar{\Gamma}_{\text{cl}} + \bar{\Gamma}, \quad (2.10b)$$

where $\bar{\Gamma}_{\text{cl}} \doteq R^{-1}$. Equation (2.10b) was obtained by integrating Eq. (2.10a) across the slab and employing the boundary conditions (2.3) on $\langle T \rangle$. The term in $\bar{\Gamma}_{\text{cl}}$ is the classical or laminar contribution. It is sometimes useful to write the result (2.10b) in terms of the number N , defined as the ratio of the spatially averaged advective flux to its laminar value:

$$N \doteq \bar{\Gamma} / \bar{\Gamma}_{\text{cl}}. \quad (2.11)$$

Thus,

$$\Gamma_{\text{tot}} = R^{-1}(1 + N).$$

Note, from Eqs. (2.10a) and (2.8), that the total flux is proportional to the gradient of the mean profile at the boundary,

$$\Gamma_{\text{tot}} = -R^{-1} \langle T \rangle'(0) = -R^{-1} \langle T \rangle'(1), \quad (2.12)$$

and thus that

$$N = -\langle T \rangle'(0) - 1 = -\langle T \rangle'(1) - 1.$$

From Eq. (2.10b) we see that the spatial average $\bar{\Gamma}$ of the advective flux is of crucial importance, since $\bar{\Gamma}_{cl}$ is known. Either by directly averaging Eq. (2.4) according to Eq. (2.7) or by employing Eq. (2.6) to evaluate Eq. (2.12), one finds

$$\Gamma(x) = \bar{\Gamma} + R^{-1} \left(1 - \left\langle \left(\frac{1}{2} Ru \right) \frac{\cosh(Ru(x - \frac{1}{2}))}{\sinh(\frac{1}{2} Ru)} \right\rangle \right), \quad (2.13)$$

where

$$\bar{\Gamma} = R^{-1} \left[\left\langle \left(\frac{1}{2} Ru \right) \coth\left(\frac{1}{2} Ru\right) \right\rangle - 1 \right] \quad (2.14a)$$

$$\sim \begin{cases} \frac{1}{12} R - \frac{1}{240} R^3 & (R \rightarrow 0), \\ (2\pi)^{-1/2} \approx 0.40 & (R \rightarrow \infty). \end{cases} \quad (2.14b)$$

The limit of small R describes the hydrodynamic quasilinear scaling (1.12c). The general quasilinear formalism is reviewed in Sec. 5.1, where we rederive the factor of $1/12$. Of course, the limit of large R reproduces the strong turbulence scaling (1.12d). Also note that the result (2.6) is compatible with the integration of Eqs. (2.10) using Eq. (2.13).

Representative spatial profiles of the advective flux $\Gamma(x)$ are displayed in Fig. 5. Note the boundary layer phenomenon for large R . The width Δ of each boundary layer is of order R^{-1} . This can be seen explicitly from examination of Eq. (2.13). However, it can also be estimated by simple (and more general) arguments of flux continuity. Reverting temporarily to dimensional units, we can argue as follows. In the interior, the flux is advective, with characteristic velocity $\bar{u}$. However, because of the boundary conditions the flux through the boundary must be carried entirely classically, with diffusion velocity κ/Δ . By continuity, these must balance at the edge of the boundary layer:

$$\kappa/\Delta \sim \bar{u},$$

or

$$\Delta/L \sim R^{-1} = \bar{\Gamma}_{cl}.$$

The dependences of Γ_{tot} , $\bar{\Gamma}$, $\bar{\Gamma}_{cl}$, and N on the Reynolds number are shown in Fig. 6. The advective and classical components are equal for Reynolds number R_1 , where $N(R_1) = 1$. The value of R_1 can be obtained numerically (we used *regula falsi* iteration), and is

$$R_1 \approx 4.32.$$

This is indicated graphically by the dotted lines in Fig. 6. At this point,

$$\bar{\Gamma}_{cl} = \bar{\Gamma} = R_1^{-1} \approx 0.23.$$

Thus, the limiting value (2.14b) for $\bar{\Gamma}$ is about twice the transition value. The total flux Γ_{tot} is approximately constant for $N > 1$.

2.3 Variational principle for the basic constraint

For practical applications, the fundamental dynamical description typically consists of complicated integro-differential equations for which exact solutions are unavailable. Thus, approximate techniques are required. In this section we shall derive the variational principle and apply it to the reference model. It is possible here to consider a slight generalization of Eq. (2.1), in which we allow for temporal, though still not spatial (see Sec. 3), dependence of u (that is, we allow K to be finite):

$$\frac{\partial}{\partial t} T(x, t) + u(t) \frac{\partial T}{\partial x} - R^{-1} \frac{\partial^2 T}{\partial x^2} = 0, \quad (2.15)$$

again with the boundary conditions Eq. (2.3). We shall call Eq. (2.15) the *generalized reference model*; it is described by a finite Kubo number, in addition to R . In fact, as we will see, the time dependence of u will not enter into the calculations of this section. However, in Sec. 5 we will generalize the formalism to explicitly include a finite K .

We shall consider Eq. (2.15) only in the statistically steady state. Therefore, the flux conservation relations (2.10) remain unchanged. Consider now the equation for the concentration fluctuation:

$$\frac{\partial}{\partial t} \delta T(x, t) + \delta u(t) \frac{\partial}{\partial x} \langle T \rangle + \frac{\partial}{\partial x} (\delta u \delta T - \langle \delta u \delta T \rangle) - R^{-1} \frac{\partial^2}{\partial x^2} \delta T = 0. \quad (2.16)$$

Let us define the “energy” by

$$\mathcal{E}(x) \doteq \frac{1}{2} \langle \delta T^2 \rangle.$$

The energy balance equation is formed by multiplying Eq. (2.16) by $\delta T(x, t)$ [at the same time and space point as that of Eq. (2.16)] and ensemble-averaging. In order to write the resulting equation in a suggestive form, let us define also the *production* term

$$\mathcal{P}(x) \doteq -\Gamma(x) \frac{d}{dx} \langle T \rangle(x) \quad (2.17)$$

[where Γ is defined by Eq. (2.7)], the *transfer* term

$$\mathcal{T}(x) \doteq \frac{1}{2} \frac{d}{dx} \langle \delta u \delta T^2 \rangle, \quad (2.18)$$

and the *dissipation* term

$$\begin{aligned} \mathcal{D}(x) &\doteq -R^{-1} \left\langle \delta T \frac{\partial^2}{\partial x^2} \delta T \right\rangle \\ &= R^{-1} \left\langle \left(\frac{\partial \delta T}{\partial x} \right)^2 \right\rangle. \end{aligned} \quad (2.19)$$

(We integrated by parts and used the boundary conditions.) Then we obtain

$$\frac{d}{dt}\mathcal{E}(x) = \mathcal{P}(x) - \mathcal{T}(x) - \mathcal{D}(x).$$

Equations of this type are well known in fluid dynamics.²⁸ In the statistically steady state, all quantities are stationary, and we arrive at our prototypical balance equation:

$$\mathcal{P}(x) = \mathcal{T}(x) + \mathcal{D}(x). \quad (2.20)$$

Because of expression (2.18), we have here the familiar closure problem: To proceed exactly, one needs to evaluate the triplet correlation $\langle \delta u \delta T^2 \rangle$, an expression for which is not immediately available. In Sec. 4, we will for completeness show how to approximate this term by using the direct-interaction approximation. However, in the optimum theory one proceeds differently. In this method, one notes that the conservative nature of Eq. (2.15) ensures that the transfer term will be a divergence, as can be seen explicitly in definition (2.18). We may exploit this fact to *annihilate* the triplet correlation by integrating Eq. (2.20) across the layer, using the boundary conditions $\delta T(0) = \delta T(1) = 0$. We obtain

$$\overline{\mathcal{P}} = \overline{\mathcal{D}}. \quad (2.21)$$

With suitable interpretations of $\mathcal{P}$ and $\mathcal{D}$, this equation remains valid in general, not just for the reference model. It is this expression of the global balance between production and dissipation on which the variational principle will be built.

Equation (2.21) is not in optimal form, however. The mean concentration gradient which occurs in the production term is not yet determined, as it is self-consistently related to the flux through the continuity equation. Although we could work with both mean and fluctuating fields and impose the continuity relation as an additional constraint, it is more convenient to work from the start in a manifold consisting of fluctuating fields only. To this end, let us define

$$\Delta\Gamma \doteq \Gamma(x) - \overline{\Gamma} \quad (2.22)$$

and write Eq. (2.10) in the form

$$-\frac{d}{dx}\langle T \rangle(x) = 1 - R\Delta\Gamma(x). \quad (2.23)$$

We may use this equation to eliminate the mean concentration gradient from (2.18), finally re-expressing Eq. (2.21) in the form

$$\overline{\Gamma} = R^{-1}\overline{|\delta T'|^2} + R\overline{\Delta\Gamma^2}. \quad (2.24)$$

Here $\delta T' \doteq \partial\delta T/\partial x$. To obtain the second term on the right-hand side of Eq. (2.24), we used the identity $\overline{\Gamma\Delta\Gamma} = \overline{\Delta\Gamma^2}$, which holds because $\overline{\Delta\Gamma} \equiv 0$. This term may be interpreted as the dissipation associated with a generalized Reynolds stress. Equation (2.24) describes

an intimate relation between transport and dissipation, and may be considered to be a nonlinear (in δT) constraint on the mean flux. Note that this constraint ensures that $\bar{\Gamma}$ is positive (*i.e.*, in the direction opposite to that of the concentration gradient).

We may now state the basic variational problem:

$$\text{Maximize the functional } \bar{\Gamma}\{\delta T\} \text{ subject to the constraint (2.24).} \quad (2.25)$$

For this problem of passive advection, the variation is to be done for fixed probability distribution $P(u)$, so only the concentration field $\delta T(x; u)$ is to be varied. In Appendix A, we describe in detail the variational operation of functional differentiation with respect to δT .

Before performing the variation explicitly, it is instructive to ask qualitatively whether Eq. (2.24) is sufficient to generate a well-posed problem. By noting from Eq. (2.24) that $\bar{\Gamma}$ is positive definite and then using Schwartz' inequality, we have

$$\bar{\Gamma} = |\bar{\Gamma}| = |\langle \delta u \delta T \rangle| \leq \langle \delta u^2 \rangle^{1/2} \langle \delta T^2 \rangle^{1/2} = \langle \delta T^2 \rangle^{1/2}. \quad (2.26)$$

Since the right-hand side of Eq. (2.24) scales as δT^2 whereas Eq. (2.26) scales as δT , it is impossible to either increase (or decrease) $|\delta T|$ without bound and still satisfy the constraint. Similarly, one cannot increase without bound the mean-squared gradient, while holding δT fixed. It is possible to increase the gradient while reducing δT , but if δT is reduced too far, one loses the effect of the positive-definite term in $\Delta \Gamma^2$. Thus, in the optimum solution both terms of Eq. (2.24) contribute competitively to the final maximum. It is easy to see that as $R \rightarrow \infty$ that competition will lead to the formation of boundary layers of width of order R^{-1} .

A straightforward algebraic implementation of the optimum principle would emerge by studying the unconstrained maximum of the functional

$$\mathcal{G}\{\delta T; \lambda\} \doteq \bar{\Gamma} + \lambda \left(\bar{\Gamma} - R^{-1} |\delta T'|^2 - R \Delta \Gamma^2 \right), \quad (2.27)$$

where λ is a Lagrange multiplier. Although this calculation is quite feasible (it is sketched in Appendix B), it is slightly awkward because of the need to determine λ . This annoyance is usually compounded in the self-consistent problems. However, Howard has shown⁵ how to reformulate the problem as a homogeneous minimum principle, in which the Lagrange multiplier does not appear explicitly. (It vanishes at the minimum.) To describe this procedure, we rewrite Eq. (2.24) as

$$R = \frac{|\delta T'|^2 + R^2 \Delta \Gamma^2}{\bar{\Gamma}}. \quad (2.28)$$

As it stands, the right-hand side of Eq. (2.28) is not homogeneous in δT . However, consider the following homogeneous functional $\mathcal{R}$ of δT , constructed from Eq. (2.28) and parametrized by a positive constant γ :

$$\mathcal{R}\{\delta T; \gamma\} \equiv \mathcal{R}(\gamma) \doteq \gamma \left(\frac{|\overline{\delta T}|^2 + R^2 \overline{\Delta \Gamma^2}}{\overline{\Gamma}^2} \right). \quad (2.29)$$

We then have the following principle, which can be shown to be equivalent to (2.25): *For fixed γ ,*

$$\text{Minimize } \mathcal{R}(\gamma) \text{ subject to } \overline{\Gamma} = \gamma. \quad (2.30)$$

By inverting the relation $R = \mathcal{R}_{\min}(\gamma)$, one obtains the bounding curve $\gamma(R)$ describing the maximum flux γ for a fixed R .

We shall call the constraint

$$\overline{\Gamma} = \gamma \quad (2.31)$$

the “physical normalization.” Indeed, under the physical normalization Eq. (2.29) reproduces the basic constraint (2.24). To complete the proof of the equivalence of the minimum principle (2.30) to the original maximum principle (2.25), one must show that the minimizing $\mathcal{R}(\gamma)$ is monotonic. The proof follows that of Busse,⁶ and we shall not repeat it here. Alternatively, one can demonstrate the equivalence directly by comparing the Euler equations derived from Eqs. (2.27) and (2.29). This is done in Appendix B.

The Euler equation which describes the stationary point of Eq. (2.29) is

$$-\delta T''(x) + R^2 u \Delta \Gamma(x) = (\overline{\Gamma}/\gamma) \mathcal{R}u. \quad (2.32)$$

Since we are describing the minimizing solution, we are entitled to set $\mathcal{R} = R$. Equation (2.32) is linear in δT ; this is a special feature of the passive problems which does not persist in the self-consistent ones. Also, note that the Euler equation is homogeneous in δT (since both Γ and $\overline{\Gamma}$ are of first order in δT), so it is not necessary at this stage to impose the physical normalization $\overline{\Gamma} = \gamma$. Any nonzero normalization will lead to the same response relationship $\gamma(R)$. (This feature does persist self-consistently.) Although there is no compelling technical reason not to choose the physical normalization in the passive problem, nonphysical normalizations are often extremely useful in the self-consistent problems. Thus, for pedagogical purposes we shall choose here an arbitrary normalization. Let daggers denote quantities corresponding to the nonphysical normalization

$$\overline{\Gamma}^\dagger = \alpha \gamma, \quad (2.33)$$

for arbitrary nonvanishing α . Then we must solve the (now inhomogeneous) Euler equation

$$-\delta T^{\dagger''}(x) + R^2 u \Delta \Gamma^\dagger(x) = \alpha R u. \quad (2.34)$$

This can be done by forming an equation for the flux $\Gamma^\dagger(x)$. This is simple for the reference model because u is independent of x and thus commutes with the spatial derivatives; we generalize the technique in the next section. Thus, upon multiplying Eq. (2.34) by u , ensemble-averaging, and using Eqs. (2.22) and (2.33), we obtain

$$-\Gamma^{\dagger\prime\prime}(x) + R^2 \Gamma^\dagger(x) = aR^2(\gamma + R^{-1}), \quad (2.35)$$

the solution of which, under the boundary conditions (2.3), is

$$\Gamma^\dagger(x) = a(\gamma + R^{-1})\hat{\Gamma}(x; R), \quad (2.36)$$

where

$$\hat{\Gamma}(x; R) \doteq 1 - \phi(x; R) \quad (2.37)$$

and

$$\phi(x; R) \doteq \frac{\cosh(R(x - \frac{1}{2}))}{\cosh(\frac{1}{2}R)}. \quad (2.38)$$

Now we bar Eq. (2.37) and assert the chosen nonphysical normalization (2.38). We obtain

$$a\gamma = a(\gamma + R^{-1})(1 - \Phi),$$

where

$$\Phi \equiv \bar{\Phi}(R) \doteq \int_0^1 d\bar{x} \phi(\bar{x}; R);$$

one finds

$$\Phi(z) = 2 \tanh(\frac{1}{2}z)/z \quad (2.39a)$$

$$\sim \begin{cases} 1 - \frac{1}{12}z^2 & (z \ll 1), \\ 2/z & (z \gg 1). \end{cases} \quad (2.39b)$$

As it must, the arbitrary constant a cancels out. We are left with an equation relating γ and R , which can be readily solved to yield the basic bound:

$$\gamma = \gamma_\infty(R) \doteq R^{-1} \left(\frac{1 - \Phi}{\Phi} \right) \quad (2.40a)$$

$$= R^{-1} [(\frac{1}{2}R) \coth(\frac{1}{2}R) - 1] \quad (2.40b)$$

$$= \begin{cases} \frac{1}{12}R - \frac{1}{720}R^3 & (R \rightarrow 0), \\ \frac{1}{2} & (R \rightarrow \infty). \end{cases} \quad (2.40c)$$

The physical normalization ensures us that $\gamma(R)$ is the bound $\bar{\Gamma}_{\max}$ on the true solution $\bar{\Gamma}$.

The bound (2.40) is compared with the exact solution (and with the result of the direct-interaction approximation; see Sec. 4) in Fig. 7. The bound is worst, although quite

acceptable, as $R \rightarrow \infty$. There, the relative error is $\sqrt{\pi/2} - 1 \approx 25\%$. For $R \rightarrow 0$, the relative error in the slopes vanishes; all theories reduce to the hydrodynamic quasilinear result in this limit. Differences first appear in the term of $\mathcal{O}(R^3)$, for which the relative error in the coefficient is $2/3 \approx 67\%$. We shall discuss the direct-interaction approximation in detail in Sec. 4. Here, let us just remark that although that approximation clearly produces a better estimate of the correct result, it requires considerably more labor. Furthermore, it evidently does not provide an upper bound.

Spatial profiles of $\Gamma(x)$ are compared in Figs. 8 and 9. The bounding flux reproduces the essential features of the exact solution. For large R , the flux is essentially flat at its mean value, except for the boundary layers. This behavior is evident from the analytic result (2.37).

Comparison of Eq. (2.40b) with the exact solution Eq. (2.4) reveals that they are very closely related. Indeed, the bounding result can be obtained from the exact one by replacing the given, Gaussian distribution $P(u)$ by the unique normalized distribution concentrated at $|u| = 1$, namely

$$P_v(u) \doteq \frac{1}{2}[\delta(u+1) + \delta(u-1)]. \quad (2.41)$$

This is the distribution which appears, at order 2, in the theory of Gaussian integration³³ with respect to the weight $P(u)$. This result could have been anticipated. Using the subscript 'v' to identify the solution of the variational problem, one can use Eq. (2.23) to write Eq. (2.35) in the form

$$\frac{d}{dx} \langle T \rangle_v(x) - R^{-1} \frac{d^2}{dx^2} \Gamma_v(x) = 0,$$

which should be compared to the exact result which follows from Eq. (2.16):

$$\frac{d}{dx} \langle T \rangle(x) + \frac{d}{dx} \langle \delta u^2 \delta T \rangle(x) - R^{-1} \frac{d^2}{dx^2} \Gamma(x) = 0.$$

Thus, the optimum theory has provided a mean field theory which completely ignores the triplet correlation. Note that the unique distribution which annihilates $\langle \delta u \delta T^2 \rangle$ as well as $\langle \delta u^2 \delta T \rangle$ for arbitrary δT is just (2.41).

The close connection between mean field theory and the optimum theory has been noticed before. In the self-consistent problems, the Euler-Lagrange equations of the basic bound are similar, though not identical, to those of mean field theory.²⁹ The exact agreement in the passive problems arises because the advecting field is not allowed to respond to perturbations.

Again, we point out that only the equal-time properties of u entered this calculation. Thus, the Kubo number does not appear in the result for the basic bound. Though rigorous, the basic bound fails to capture important aspects of the physics. We shall improve the calculation in Sec. 5.

2.4 The case of specified concentration gradient

Finally, let us ask how the variational calculation would be modified if one assumed that the mean concentration gradient were a fixed number. In this case the continuity equation may not be used, and the global balance (2.21) reduces to

$$\bar{\Gamma} = R^{-1} \overline{|\delta T'|^2} \quad (2.42)$$

[cf. Eq. (2.24)]. One may imagine attempting to maximize $\bar{\Gamma}$ by scaling δT with a parameter ζ ; in order to satisfy Eq. (2.42), one must simultaneously increase the characteristic spatial scale x according to $x \sim \zeta^{1/2}$. However, the longest spatial scale is restricted to the width L of the layer, which is proportional to R . Thus, $\zeta \sim R^2$ and $\delta T' \sim \zeta/L \sim R$, so we estimate the bounding flux for constant gradient to be $\gamma \sim R$. Unlike our earlier solution (2.40c), this result does not saturate, but rather diverges as $R \rightarrow \infty$. This is because the competition described in the paragraph following Eq. (2.26) is absent, so that boundary layers do not form.

To obtain a quantitative answer, one may solve the Euler equation which follows from Eq. (2.42). This equation may be obtained from Eq. (2.34) by omitting the term in $\Delta\Gamma$. The solution is

$$\Gamma(x) = \frac{1}{2} R x (1 - x), \quad (2.43a)$$

$$\gamma = \gamma_h \doteq \frac{1}{12} R, \quad (2.43b)$$

just the hydrodynamic flux. When the dissipation is very small, this flux is very large and is not a useful estimate of the strong turbulence result $\gamma \sim 1$ which obtains when the gradient is allowed to adjust self-consistently. Notice also that Eq. (2.43a) does not agree with the prediction of the continuity equation, which for the case of constant gradient would say that $\Gamma(x)$ would be constant.

In this passive version of the constant gradient calculation, we obtain for fixed R a finite bound. The situation is worse for self-consistent problems. Equation (2.42) still holds, but now both sides are of second degree in undetermined fluctuating quantities. Assuming that $\delta u \propto \delta T$, one may scale δT arbitrarily without violating Eq. (2.42). Thus, $\bar{\Gamma}$ can be made as large as one pleases, and the self-consistent basic bound for fixed mean gradient is infinity.

3. GENERAL FORMALISM FOR THE BASIC CONSTRAINT

Now we shall consider the extent to which the assumptions of the reference model can be relaxed. In particular, we shall consider the possibilities of several dimensions, spatial dependence of u , and a dissipation operator more general than $-\kappa d^2/dx^2$. The

fundamental equation is essentially Eq. (1.1). However, for future convenience (in Sec. 3.1 only), we choose to write it in a slightly different notation:

$$\frac{\partial}{\partial t} T(\mathbf{x}, t) + \nabla \cdot [\mathbf{u}(\mathbf{x}, t) T] + \hat{R}^{-1} \hat{\mathcal{L}} T = 0; \quad (3.1)$$

we shall require

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

In Eq. (3.1), the quantity $\hat{R}$ is just the Reynolds number of Eq. (1.3). Shortly, however, we will introduce a slightly different normalization which will prove more convenient, as it will enable us to derive formulas, in terms of new quantities R and $\mathcal{L}$, which will be identical in form to some of those in Sec. 2.

It is useful to define a scalar product by the combination of layer- and ensemble-averaging:

$$\langle a | b \rangle \doteq \int_0^1 dx \langle a(\mathbf{x}) b(\mathbf{x}) \rangle.$$

(This scalar product is not the same as the generalized barring operation which we will introduce shortly.) We shall assume that $\hat{\mathcal{L}}$ is a linear, formally self-adjoint,³⁴ positive-definite operator and that the boundary conditions on δT are self-adjoint³⁴ as well, so that

$$\langle \delta \psi | \hat{\mathcal{L}} | \delta \psi \rangle > 0 \quad (3.2)$$

for arbitrary normalizable $\delta \psi$. The dissipative property (3.2) is required in order that steady states can be achieved. Furthermore, we shall assume that $\hat{\mathcal{L}}$ can be written in conservation form, so that a statement of flux conservation similar to Eq. (2.10) still holds. Physically, this means that we allow no sources within the region, either completely independent of T or proportional to some power of T . (An example of an important physical effect which is not allowed is Ohmic heating of a magnetically confined plasma; see Sec. 7 for further discussion.) We shall denote the Fourier transform of $\hat{\mathcal{L}}$ with respect to the homogeneous directions by $\hat{\mathcal{L}}_k$. Note that $\hat{\mathcal{L}}\langle A \rangle = \hat{\mathcal{L}}_0\langle A \rangle$.

The most concise way of generalizing the results of Sec. 2, for quite general boundary conditions and form of $\hat{\mathcal{L}}$, is to employ the full power of the theory of Green's functions³⁴; the price paid is a certain loss of specificity. Thus, we shall develop the generalization in two steps. First, in Sec. 3.1 we shall restrict our consideration to dissipation operators of second order in x and to the simplest (and probably most physical) boundary conditions

$$\begin{aligned} \langle T(0) \rangle &= 1, \\ \langle T(1) \rangle &= 0. \end{aligned} \quad (3.3)$$

Unlike the calculations in Sec. 2, at this point we make no assumption other than self-adjointness about the boundary conditions on δT . Given these assumptions, we shall develop and discuss the appropriate generalization of the variational principle. Then, in the final generalization we shall in Sec. 3.2 briefly describe the formulas which follow from a complete Green's function treatment. Such results may be required for higher order operators in x , or for unusual, possibly mixed, boundary conditions on $\langle T \rangle$ and its derivatives.

3.1 Second order operators

The assumptions about $\hat{\mathcal{L}}$ imply that, when $\hat{\mathcal{L}}$ is second order in x , the most general operator $\hat{\mathcal{L}}_0$ which acts on ensemble-averaged quantities has the form

$$\hat{\mathcal{L}}_0 = -\frac{d}{dx}\hat{\kappa}(x)\frac{d}{dx}, \quad (3.4)$$

where $\hat{\kappa}(x) > 0$. As usual, we define

$$\Gamma(x) \doteq \langle \delta T(\mathbf{x}, t) \delta u_x(\mathbf{x}, t) \rangle;$$

we also introduce the velocity correlation function

$$U(x; x') \doteq \langle \delta u_x(\mathbf{x}, t) \delta u_x(\mathbf{x}', t) \rangle.$$

In steady state, the ensemble average of Eq. (3.1) reduces to

$$\frac{d}{dx}\Gamma(x) - \hat{R}^{-1}\frac{d}{dx}\hat{\kappa}(x)\frac{d}{dx}\langle T \rangle(x) = 0.$$

The total flux through the system is

$$\Gamma_{\text{tot}} = -\hat{R}^{-1}\hat{\kappa}(x)\frac{d}{dx}\langle T \rangle(x) + \Gamma(x) = \text{const.} \quad (3.5)$$

Given the boundary conditions (3.3), one may relate the constant of integration to the spatially averaged advective flux by dividing Eq. (3.5) by $\hat{\kappa}(x)$, then integrating from 0 to 1. This suggests a generalization of the barring operation, introduced previously, to

$$\bar{A} \doteq \int_0^1 dx \langle A \rangle(x) / \kappa(x),$$

where

$$\kappa(x) \doteq \hat{\kappa}(x) / \bar{K}$$

and

$$1/\bar{K} \doteq \int_0^1 dx / \kappa(x).$$

One can then readily see that the natural quantities are not $\hat{R}$, $\hat{\kappa}$, and $\hat{\mathcal{L}}$, but rather $\kappa(x)$,

$$R \doteq \hat{R} / \bar{K},$$

and

$$\mathcal{L} \doteq \hat{\mathcal{L}} / \bar{K},$$

such that

$$\mathcal{L}_0 = -\frac{d}{dx} \kappa(x) \frac{d}{dx}$$

and

$$\bar{\kappa} = 1.$$

Then, upon barring Eq. (3.5), we find

$$\Gamma_{\text{tot}} = R^{-1} + \bar{\Gamma}$$

as before [see Eq. (2.10b)], and

$$-\kappa(x) \frac{d}{dx} \langle T \rangle(x) = 1 - R \Delta \Gamma$$

[cf. Eq. (2.23)]. From the fluctuating part of Eq. (3.1), we find the constraint

$$\bar{\Gamma} = R^{-1} \overline{\delta T \kappa \mathcal{L} \delta T} + R \overline{\Delta \Gamma^2} \quad (3.6)$$

[cf. Eq. (2.24)]. The variational principle becomes: *Minimize the functional*

$$\mathcal{R}(\gamma) \doteq \gamma \left(\frac{\overline{\delta T \kappa \mathcal{L} \delta T} + R^2 \overline{\Delta \Gamma^2}}{\bar{\Gamma}^2} \right) \quad (3.7)$$

subject to $\bar{\Gamma} = \gamma$. The Euler equation is

$$\kappa(x) \mathcal{L} \delta T(x) + R^2 \nu(x) \Delta \Gamma(x) = R u(x), \quad (3.8)$$

where we write $u \equiv u_x$ and use immediately the physical normalization. (We shall not continue to indicate the parametric dependence of $\delta T_{\mathbf{k}}$ and $u_{\mathbf{k}}$ on time.) This equation may be most conveniently solved by first Fourier-transforming in the homogeneous directions:

$$\mathcal{L}_{\mathbf{k}} \delta T_{\mathbf{k}}(x) = -R^2 \kappa^{-1}(x) u_{\mathbf{k}}(x) [\Gamma(x) - (\gamma + R^{-1})]. \quad (3.9)$$

Because u now depends on x and does not commute with $\mathcal{L}_{\mathbf{k}}$, we cannot derive an equation for the flux by simply multiplying by u as we did in Sec. 2. Instead, we introduce Green's function $G^{(0)}$ for $\mathcal{L}$ corresponding to the (here unspecified) boundary conditions on δT . [The "0" superscript is used to distinguish this quantity from the renormalized infinitesimal response function G which appears in the direct-interaction approximation (see Sec. 4) and other renormalized closures.] Then, the solution of Eq. (3.9) is

$$\delta T_{\mathbf{k}}(x) = \mathcal{J}_{\mathbf{k}}(x) - R^2 \int_0^1 d\bar{x} G_{\mathbf{k}}^{(0)}(x; \bar{x}) \kappa^{-1}(x) u_{\mathbf{k}}(\bar{x}) [\Gamma(\bar{x}) - (\gamma + R^{-1})], \quad (3.10)$$

where

$$\mathcal{J}_{\mathbf{k}}(x) \doteq \mathcal{J}[G_{\mathbf{k}}^{(0)}(x; \xi), \delta T_{\mathbf{k}}(\xi)]_{\xi=0}^{\xi=1}$$

and where $\mathcal{J}[u, v]$, the conjunct³⁴ of u and v , is, for the second-order problem at hand,

$$\mathcal{J}[u, v](\xi) = \kappa(\xi)[u(\xi)v'(\xi) - v(\xi)u'(\xi)].$$

$\mathcal{J}_k(x)$ vanishes for the simplest boundary conditions $\delta T(0) = \delta T(1) = 0$.

Now, upon noting that

$$\Gamma(x) = \sum_k \langle \delta T_k(x) \delta u_k^*(x) \rangle,$$

we can form an integral equation for the advective flux by multiplying Eq. (3.10) by $u_k^*(x)$ and ensemble-averaging. Define an integral operator $\mathbf{M}$ whose kernel³⁵ is

$$\langle x | \mathbf{M} | x' \rangle \equiv M(x; \bar{x}) \doteq \sum_k G_k^{(0)}(x; \bar{x}) U_k(x; \bar{x}) \kappa(\bar{x}),$$

and vectors (in function space) Γ , $\mathbf{m}$, and $\mathbf{r}$ whose components are $\Gamma(x)$,

$$m(x) \doteq \int_0^1 d\bar{x} M(x; \bar{x}),$$

and

$$r(x) \doteq \sum_k \langle u_k^*(x) \mathcal{J}_k(x) \rangle.$$

Then one finds from Eq. (3.10) the linear, inhomogeneous integral equation

$$(\mathbf{I} + R^2 \mathbf{M}) \Gamma = (\gamma + R^{-1}) R^2 \mathbf{m} + \mathbf{r}, \quad (3.11)$$

with $\gamma = \bar{\Gamma}$. This may be solved by linear superposition as follows. Introduce a fundamental solution χ which solves

$$(\mathbf{I} + R^2 \mathbf{M}) \chi = R^2 \mathbf{m} \quad (3.12a)$$

or

$$(\mathbf{I} + R^{-2} \mathbf{M}^{-1}) \chi = \mathbf{1} \quad (3.12b)$$

[note the distinction between the identity operator $\mathbf{I}$, whose kernel is $\langle x | \mathbf{I} | x' \rangle = \delta(x - x')$, and the function $\mathbf{1}$, whose components are identically the number 1: $\langle x | \mathbf{1} \rangle = 1$], and also a quantity Γ_r , which obeys

$$(\mathbf{I} + R^2 \mathbf{M}) \Gamma_r = \mathbf{r}. \quad (3.13)$$

The solution to Eq. (3.11) is then

$$\Gamma(x) = \chi(x) \Gamma_{\text{tot}} + \Gamma_r(x), \quad (3.14a)$$

where

$$\Gamma_{\text{tot}} = \left(\frac{\bar{\Gamma}_{\text{cl}} + \bar{\Gamma}_r}{1 - \bar{\chi}} \right) \quad (3.14b)$$

($\bar{\Gamma}_{\text{cl}} \doteq R^{-1}$), and

$$\bar{\Gamma} = \left(\frac{\bar{\chi}}{1 - \bar{\chi}} \right) \bar{\Gamma}_{\text{cl}} + \left(\frac{1}{1 - \bar{\chi}} \right) \Gamma_r. \quad (3.14c)$$

The form of these equations is reminiscent of dielectric response in a polarizable medium, with $-\chi$ playing the role of the susceptibility. Thus, the total flux is “driven” by the dissipation, measured by $\bar{\Gamma}_{\text{cl}}$, and by the “source flux” Γ_r . The latter quantity measures the amount of advective flux specified at the boundaries. Both $\bar{\Gamma}_{\text{cl}}$ and Γ_r (or, more primitively, r) play the role of external forcing functions to which the system statistically responds in a stochastically self-consistent way. The magnitude of the response is measured by the dielectric-like quantity $1 - \bar{\chi}$. Of course, $\bar{\chi}$ is a constant number, not a function of wave number and frequency. It is most closely analogous to the long wavelength, low frequency limit of the susceptibility.

The asymptotic scalings with R of the flux can be deduced easily by examining the above equations. Let us ignore boundary contributions for simplicity. Then, for $R \rightarrow 0$ one finds $\bar{\chi} \sim R^2$, so that

$$\begin{aligned} \bar{\Gamma} &\sim R, \\ \Gamma_{\text{tot}} &\sim R^{-1} = \bar{\Gamma}_{\text{cl}}. \end{aligned} \quad (R \rightarrow 0)$$

In the limit $R \rightarrow \infty$, one finds $\bar{\chi} \sim 1 + \mathcal{O}(R^{-1})$ (the correction describes the width of the boundary layer) and recovers the strong turbulence scalings

$$\bar{\Gamma} \sim \Gamma_{\text{tot}} \sim 1. \quad (R \rightarrow \infty)$$

Of course, these results are in agreement with those for the reference model. Note that the response does not vanish as $\bar{\Gamma}_{\text{cl}} \rightarrow 0$ ($R \rightarrow \infty$). This situation is loosely analogous to the excitation of a normal mode in a dielectric medium, whereby an infinitesimal disturbance leads to a finite response at the resonant frequency. There is no sharp resonance here, so the best normal mode analogy is to the excitation of zero-frequency fluctuations—in plasmas, the so-called convective cells.³⁰

Equations of the form (3.12) are amenable to various forms of numerical solution. Since $M(x; \bar{x})$ is a known function (assuming that $G_k^{(0)}$ can be found either analytically or numerically, which will be the case for simple geometries and boundary conditions), the most straightforward technique is to write Eq. (3.12) in finite-differenced form and to treat it as a linear system; that can be solved by standard routines. A similar calculation is performed in Sec. 4 in the course of solving the direct-interaction approximation.

3.2 Higher order operators; general boundary conditions

Details of the method become somewhat tedious for dissipation operators of order higher than two, or for general boundary conditions on $\langle T \rangle$ and its derivatives. In attempting to derive principles for such situations, the first step is to determine what quantity to maximize. One must search for an appropriate generalized spatial integral $\bar{\Gamma}$ of $\Gamma(x)$ which is related to the total flux through the system by an additive expression (such as $\bar{\Gamma}_{cl} \doteq R^{-1}$) known entirely in terms of the given boundary data. [In this section, we do not use the carat notation introduced in Eq. (3.1).] The result may not be immediate. Consider, for example,

$$\mathcal{L} \doteq \kappa \frac{d^4}{dx^4},$$

with boundary conditions

$$\begin{aligned} \langle T \rangle(0) &= 1, & \langle T \rangle'(0) &= 0, \\ \langle T \rangle(1) &= 0, & \langle T \rangle'(1) &= 0. \end{aligned} \quad (3.15)$$

The continuity equation has the first integral

$$\Gamma_{tot} = \Gamma(x) + \kappa \frac{d^3}{dx^3} \langle T \rangle(x) = \text{const.}$$

A true relationship is

$$\Gamma_{tot} = \int_0^1 d\bar{x} \Gamma(\bar{x}) + \kappa \left. \frac{d^2}{dx^2} \langle T \rangle \right|_0^1,$$

but the boundary value term is not known from the boundary conditions. Rather, for each R the second derivatives will adjust themselves, in an unknown way, so that Eqs. (3.15) are satisfied. Thus, maximizing $\bar{\Gamma}^\dagger \doteq \int_0^1 d\bar{x} \Gamma(\bar{x})$ gives no immediate bound on the total flux. (However, had we specified $\langle T \rangle''$ instead of $\langle T \rangle'$, maximizing $\bar{\Gamma}^\dagger$ would have been natural.)

For the case where $\Gamma(x)$ vanishes on the boundary, we shall now indicate a general procedure whereby one can systematically construct the appropriate quantity to maximize. The mean continuity equation is

$$\frac{d}{dx} \Gamma(x) + R^{-1} \mathcal{L}_0 \langle T \rangle(x) = 0. \quad (3.16)$$

In order to make the conservation property of $\mathcal{L}_0$ explicit, let us define a new linear operator $\mathcal{L}_{cl}$ by

$$\mathcal{L}_0 \doteq -\frac{d}{dx} \mathcal{L}_{cl}.$$

(For example, for the reference model $\mathcal{L}_{cl} = d/dx$.) Then Eq. (3.16) takes the form

$$\frac{d}{dx} [\Gamma_{cl}(x) + \Gamma(x)] = 0, \quad (3.17)$$

where

$$\Gamma_{\text{cl}}(x) \doteq -R^{-1}L_{\text{cl}}\langle T \rangle(x). \quad (3.18)$$

The integral of Eq. (3.17) is

$$\begin{aligned} \Gamma_{\text{tot}} &= \Gamma_{\text{cl}}(x) + \Gamma(x) \\ &= \Gamma_{\text{cl}}(0) = \Gamma_{\text{cl}}(1). \end{aligned}$$

We shall seek a formula for $\Gamma_{\text{cl}}(0)$. Consider the formal solution of Eq. (3.16):

$$\langle T \rangle(x) = \mathcal{J}_0(x) - R \left(G_{\mathbf{0}}^{(0)} * \frac{\partial \Gamma}{\partial x} \right)(x), \quad (3.19)$$

where

$$\mathcal{J}_0(x) \doteq \mathcal{J}[G_{\mathbf{0}}^{(0)}(x; \xi), \langle T \rangle(\xi)]_{\xi=0}^{\xi=1}$$

and where the asterisk indicates operator multiplication (convolution). We may “evaluate” $\Gamma_{\text{cl}}(0)$ by applying L_{cl} to Eq. (3.19) according to Eq. (3.18):

$$\Gamma_{\text{cl}}(x) = -R^{-1}L_{\text{cl}}\mathcal{J}_0 + L_{\text{cl}}G_{\mathbf{0}}^{(0)} * \frac{\partial \Gamma}{\partial x}.$$

In evaluating this at $x = 0$, we must be careful to take the limit $x \rightarrow 0_+$ in order to avoid spurious delta functions.³⁴ Thus, very explicitly,

$$\begin{aligned} \Gamma_{\text{cl}}(0) = - \lim_{x \rightarrow 0_+} \left\{ R^{-1} \mathcal{J}[L_{\text{cl}}(x)G_{\mathbf{0}}^{(0)}(x; \xi), \langle T \rangle(\xi)]_{\xi=0}^{\xi=1} \right. \\ \left. + \int_0^1 d\bar{x} \left[L_{\text{cl}}(x) \frac{\partial}{\partial \bar{x}} G_{\mathbf{0}}^{(0)}(x; \bar{x}) \right] \Gamma(\bar{x}) \right\}, \quad (3.20) \end{aligned}$$

where in deriving the last term we integrated by parts. By general properties of the conjunct,³⁴ the term in $\mathcal{J}_0$ is known in terms of the specified boundary data (and derivatives of the known Green’s function). It is the generalization of the term in $\bar{\Gamma}_{\text{cl}}$ in equations such as Eq. (2.10b). Thus, the integral term in Eq. (3.20) defines a barring operation and gives the quantity $\bar{\Gamma}$ which should be maximized in order to bound the flux.

As an example, we may show how Eq. (3.20) reduces to the second-order case treated in Sec. 3.1. Letting $H(x)$ denote the Heaviside function,

$$H(x) \doteq \begin{cases} 1 & (x > 0), \\ 1/2 & (x = 0), \\ 0 & (x < 0), \end{cases}$$

we have

$$\begin{aligned}
L_{cl} &= \kappa(x) \frac{d}{dx}, \\
G_{\mathbf{0}}^{(0)}(x; x') &= H(x - x') \left(\int_0^{x'} d\bar{x}' / \kappa(\bar{x}') \right) \left(\int_x^1 d\bar{x} / \kappa(\bar{x}) \right) \\
&\quad + (x \rightarrow x'), \\
\frac{\partial}{\partial x'} G_{\mathbf{0}}^{(0)}(x; x') &= \kappa^{-1}(x') \left[\left(\int_x^1 d\bar{x} / \kappa(\bar{x}) \right) - H(x' - x) \right], \\
\frac{\partial^2}{\partial x \partial x'} G_{\mathbf{0}}^{(0)}(x; x') &= \kappa^{-1}(x) [\delta(x - x') - \kappa^{-1}(x')], \\
\mathcal{J}[G_{\mathbf{0}}^{(0)}, \langle T \rangle]_0^1 &= \left[\kappa(\xi) \frac{\partial}{\partial \xi} G_{\mathbf{0}}^{(0)}(x; \xi) \right]_{\xi=0}, \\
-\lim_{x \rightarrow 0_+} \{ R^{-1} \mathcal{J}[L_{cl} G_{\mathbf{0}}^{(0)}, \langle T \rangle] \} &= -R^{-1} \lim_{x \rightarrow 0_+} [\delta(x) - \kappa^{-1}(0)] \kappa(0) \\
&= R^{-1}, \\
-\lim_{x \rightarrow 0_+} \int_0^1 d\bar{x} \left[L_{cl}(x) \frac{\partial}{\partial \bar{x}} G_{\mathbf{0}}^{(0)}(x; \bar{x}) \right] \Gamma(\bar{x}) &= -\lim_{x \rightarrow 0_+} \int_0^1 d\bar{x} [\delta(x - \bar{x}) - \kappa^{-1}(\bar{x})] \Gamma(\bar{x}) \\
&= \int_0^1 d\bar{x} \kappa^{-1}(\bar{x}) \Gamma(\bar{x}) = \bar{\Gamma}.
\end{aligned}$$

Thus, $\Gamma_{tot} = \Gamma_{cl}(0) = R^{-1} + \bar{\Gamma}$ as before.

Now we must derive a constraint on the fluctuations, in order that a finite bound on $\bar{\Gamma}$ be obtained. Again, consider the steady-state balance equation:

$$\Gamma \frac{d}{dx} \langle T \rangle + \frac{1}{2} \frac{d}{dx} \langle \delta u \delta T^2 \rangle + \langle \delta T \mathcal{L} \delta T \rangle = 0. \quad (3.21)$$

Unlike the earlier examples in Sec. 2 and Sec. 3.1, the spatial operation to be applied to this equation is *not* the barring operation, but is rather dictated by the necessity of annihilating the triplet correlation. Under the boundary conditions $\delta T(0) = \delta T(1) = 0$, this is just the spatial integral. Thus, upon integrating Eq. (3.21) from 0 to 1 and substituting Eq. (3.19) for $\langle T \rangle$, we get

$$-\langle \mathcal{J}'_0 | \Gamma \rangle = R^{-1} \langle \delta T | \mathcal{L} | \delta T \rangle + R \left\langle \Gamma \left| \frac{d}{dx} G_{\mathbf{0}}^{(0)} \right| \frac{d\Gamma}{dx} \right\rangle;$$

several integrations by parts convert this to the more symmetric form

$$\langle \mathcal{J}_0 | \Gamma' \rangle = R^{-1} \langle \delta T | \mathcal{L} | \delta T \rangle + R \left\langle \frac{d\Gamma}{dx} \left| G_0^{(0)} \right| \frac{d\Gamma}{dx} \right\rangle. \quad (3.22)$$

Since we have assumed that $\mathcal{L}$ is positive definite, the first term on the right of Eq. (3.22) is positive. In fact, so is the second term, since we can write, for arbitrary ψ , the inequality

$$\langle \psi | \mathcal{L} | \psi \rangle > 0$$

as

$$\langle \psi | \mathcal{L} G^{(0)} \mathcal{L} | \psi \rangle > 0$$

or

$$\langle (\mathcal{L}\psi) | G^{(0)} | (\mathcal{L}\psi) \rangle > 0,$$

thus proving that $G^{(0)}$ is positive definite, since ψ is arbitrary.

We can now pose the basic variational principle for arbitrary boundary conditions on $\langle T \rangle$, unspecified self-adjoint boundary conditions on δT except that $\delta T(0) = \delta T(1) = 0$, and arbitrary self-adjoint, positive definite $\mathcal{L}$: *Minimize*

$$\mathcal{R}(\gamma) = \gamma \left(\frac{\langle \delta T | \mathcal{L} | \delta T \rangle + R^2 \left\langle \Gamma \left| \frac{\partial^2 G^{(0)}}{\partial x \partial \bar{x}} \right| \Gamma \right\rangle}{\bar{\Gamma} \langle \mathcal{J}_0 | \Gamma' \rangle} \right) \quad (3.23a)$$

subject to

$$\bar{\Gamma} = \gamma, \quad (3.23b)$$

where

$$\bar{\Gamma} \doteq - \lim_{z \rightarrow 0^+} \int_0^1 d\bar{x} \left[L_{cl}(x) \frac{\partial}{\partial \bar{x}} G_0^{(0)}(x; \bar{x}) \right] \Gamma(\bar{x}). \quad (3.23c)$$

It is readily checked that Eq. (3.23) properly reduces to Eq. (3.7).

4. THE DIRECT-INTERACTION APPROXIMATION

In this section we shall return to the reference model, in order to describe the predictions of the direct-interaction approximation for it. Our goals here are several. First, it is useful to contrast the variational procedure with more standard closure theory. Second, the relevant response functions for the reference model are entirely time-independent but spatially inhomogeneous, a situation which is not often studied in practice.

4.1 Features of the direct-interaction approximation

The direct-interaction approximation^{2,1,3} is a statistical closure theory which approximates triplet correlations by particular integral functions of two-point correlations. In field theory,¹ it corresponds to mass (line) renormalization in the absence of charge (vertex) renormalization.^{3b} An important feature of the direct-interaction approximation is that it is the exact statistical description of certain realizable statistical models,⁷ so its behavior is guaranteed to be "reasonable." The calculation which we shall perform below is closely analogous, both in intent and detail, to Kraichnan's solution for the infinitesimal response function of the stochastic oscillator.⁷

Fundamentally, the direct-interaction approximation approximates two-time- and two-space-point correlations. Although the resulting predictions are detailed, the richness of description also leads in general to equations which are technically very difficult to solve, even with the aid of supercomputers; this is especially true for inhomogeneous situations. Thus, the numerical solution of the direct-interaction approximation which we carry out below for the reference model is of some general interest.

4.2 Derivation of the direct-interaction approximation for the reference model

The derivation of the direct-interaction approximation for the reasonably general passive advection model (1.1) is described in Appendix C. There, we allow for an advecting velocity which is both a vector and a function of $\mathbf{x}$ and t . The resulting formulas are somewhat complicated. However, they simplify considerably for the reference model, where the velocity correlation tensor $\mathbf{U} \doteq \langle \delta \mathbf{u} \delta \mathbf{u} \rangle$ becomes a scalar constant,

$$\mathbf{U}(\mathbf{x}, t; \mathbf{x}', t') = 1,$$

and where the mixed correlation function $\mathbf{\Gamma} \doteq \langle \delta T \delta \mathbf{u} \rangle$ becomes a scalar function of just its first set of arguments,

$$\mathbf{\Gamma}(\mathbf{x}, t; \mathbf{x}', t') \rightarrow \Gamma(\mathbf{x}, t).$$

Furthermore, in the time-asymptotic steady state, when initial transients have died out,

$$\Gamma(\mathbf{x}, t) \rightarrow \Gamma(\mathbf{x}).$$

Thus, upon specializing Eq. (C.9) to the reference model, we find that the mean (renormalized) infinitesimal response function G obeys the Dyson equation

$$\left(\frac{\partial}{\partial \tau} + \mathcal{L} \right) G(\mathbf{x}, \tau; \mathbf{x}') + \int_0^\tau d\bar{\tau} \int_0^1 d\bar{x} \Sigma(\mathbf{x}, \bar{\tau}; \bar{\mathbf{x}}) G(\bar{\mathbf{x}}, \tau - \bar{\tau}; \mathbf{x}') = \delta(\tau) \delta(\mathbf{x} - \mathbf{x}'), \quad (4.1)$$

where

$$\mathcal{L} \doteq -R^{-1} \frac{\partial^2}{\partial x^2},$$

and

$$\Sigma(x, \tau; \bar{x}) \doteq -\frac{\partial}{\partial x} \int_0^1 dy G(x, \tau; y) \frac{\partial}{\partial y} \delta(y - \bar{x}). \quad (4.2)$$

(Here, we write Σ as an ordinary function, not, as we did in Appendix C, as an operator.) Note that the functions G and Σ are stationary in time, since $\langle \delta u^2 \rangle$ is constant. In general, the flux is nonstationary. If we allow temporarily for arbitrary time dependence arising from an initial transient, the flux obeys

$$\left(\frac{\partial}{\partial t} + \mathcal{L} \right) \Gamma(x, t) + 2 \int_0^t d\bar{\tau} \int_0^1 d\bar{x} \Sigma(x, \bar{\tau}; \bar{x}) \Gamma(\bar{x}, t - \bar{\tau}) = -\frac{\partial}{\partial x} \langle T \rangle(x, t). \quad (4.3)$$

[Note the factor of 2 in this equation relative to Eq. (4.1).] However, we are interested in the time-asymptotic situation in which initial transients have died away. In that limit, we do expect statistical stationarity, such that $\Gamma(x, t)$ becomes independent of t . Equation (4.3) is compatible with this result. Specifically, because $\Sigma(\tau)$ has a finite lifetime,

$$\lim_{t \rightarrow \infty} \int_0^t d\bar{\tau} \Sigma(\bar{\tau}) \Gamma(t - \bar{\tau}) = \left[\int_0^\infty d\bar{\tau} \Sigma(\bar{\tau}) \right] \lim_{t \rightarrow \infty} \Gamma(t).$$

It can then be seen that the equations are consistent with the result $\lim_{t \rightarrow \infty} \Gamma(x, t) = \Gamma(x)$, so that Eq. (4.3) reduces to

$$\mathcal{L}\Gamma(x) + 2 \int_0^1 d\bar{x} \left[\int_0^\infty d\bar{\tau} \Sigma(x, \bar{\tau}; \bar{x}) \right] \Gamma(\bar{x}) = -\frac{\partial}{\partial x} \langle T \rangle(x). \quad (4.4)$$

Finally, the mean concentration gradient is self-consistently related to the flux by Eq. (2.23), which we repeat for convenience:

$$-\frac{\partial}{\partial x} \langle T \rangle(x) = 1 - R \Delta \Gamma(x). \quad (4.5)$$

Noting Eq. (4.2), we see that Eq. (4.4) requires only the reduced quantity

$$G(x; x') \doteq \int_0^\infty d\tau G(x, \tau; x'),$$

the zero-frequency Fourier component of the response function. A closed equation for this quantity follows by integrating Eq. (4.1) in τ from 0_- to ∞ , then interchanging the order of time integration in the nonlinear term:

$$-R^{-1} \frac{\partial^2}{\partial x^2} G(x; x') - \int_0^1 d\bar{x} \frac{\partial}{\partial x} G(x; \bar{x}) \frac{\partial}{\partial \bar{x}} G(\bar{x}; x') = \delta(x - x'). \quad (4.6)$$

Equations such as this are familiar, in a somewhat different guise, in the theory of closures for homogeneous turbulence¹² when the two-time behavior of the DIA response function is

approximated by wave number-dependent exponential damping: $G(\tau) \approx H(\tau) \exp(-\eta_k \tau)$. The correspondence is $G(x; x') \rightarrow \eta_k^{-1}$. However, we have made no approximation in arriving at Eq. (4.6).

The solution of Eq. (4.6) can be shown to be symmetric:

$$G(x; x') = G(x'; x).$$

An alternative form of the nonlinear term, which is especially useful for the numerical work, can be obtained by integrating by parts and employing the boundary conditions

$$G(0; x') = G(1; x') = 0, \quad (4.7)$$

which are inherited³⁴ from the boundary conditions $\delta T(0) = \delta T(1) = 0$:

$$-\int_0^1 d\bar{x} \frac{\partial}{\partial x} G(x; \bar{x}) \frac{\partial}{\partial \bar{x}} G(\bar{x}; x') = \int_0^1 d\bar{x} \left[\frac{\partial^2}{\partial x \partial \bar{x}} G(x; \bar{x}) \right] G(\bar{x}; x'). \quad (4.8)$$

The bracketed term is an alternative form for $\Sigma(x; \bar{x})$ [cf. Eq. (4.2)].

4.3 Properties of the infinitesimal response function

Equation (4.6) [with Eq. (4.7)] is a nonlinear boundary value equation in two variables. Although the general structure of its spatial Fourier transform is quite similar to that of the temporal Fourier transform of the familiar stochastic oscillator,^{7,3} we have been unable to find an analytic solution in closed form. Below, we shall describe the numerical solution. First, however, it is useful to consider certain analytic results.

The behavior of G near $x = x'$ is a true cusp, not modified by the nonlinearity. This can be seen by integrating Eq. (4.6) across a small region around $x = x'$. Because G must be continuous across the source point x' and since its derivative must be piecewise-continuous, the nonlinear term does not contribute to the cusp:

$$-\int_{x'_-}^{x'_+} dx \left[\int_0^1 d\bar{x} \frac{\partial}{\partial x} G(x; \bar{x}) \right] \frac{\partial}{\partial \bar{x}} G(\bar{x}; x') = \int_0^1 d\bar{x} [G(x'_+; \bar{x}) - G(x'_-; \bar{x})] \frac{\partial}{\partial \bar{x}} G(\bar{x}; x') = 0,$$

so the jump in derivative across the cusp is determined solely by the linear term:

$$\Delta G \equiv \left. \frac{\partial}{\partial x} G(x; x') \right|_{x=x'_-}^{x=x'_+} = \Delta G^{(0)} = -R.$$

As we will see, the effect of the nonlinearity is to take account of nonlocal spatial interactions by broadening the response function toward the boundaries as R becomes large.

Let us now consider perturbation theory. In the limit of small R , the zeroth-order approximation is clearly $G \approx G^{(0)}$, where the zeroth-order Green's function $G^{(0)}$ obeys

$$-R^{-1} \frac{\partial^2}{\partial x^2} G^{(0)}(x; x') = \delta(x - x').$$

The solution of this equation is well known³⁴ to be

$$G^{(0)}(x; x') = R[H(x' - x)x(1 - x') + (x \leftrightarrow x')]. \quad (4.9)$$

It is well known that a straightforward iteration of Eq. (4.6) in powers of the nonlinearity is ill-motivated and ill-behaved.³ In order to avoid spurious secularities, it is better to approximate the inverse of the response function rather than the function itself.¹ To next order in perturbation theory, then, we should evaluate the mass operator Σ at $G^{(0)}$:

$$\begin{aligned} \Sigma(x; \bar{x}) &\approx \Sigma^{(0)}(x; \bar{x}) \\ &= \frac{\partial^2}{\partial x \partial \bar{x}} G^{(0)}(x; \bar{x}) \\ &= R[\delta(x - \bar{x}) - 1]. \end{aligned}$$

This is the so-called quasilinear approximation. The operation of $\Sigma^{(0)}$ on G is then

$$\int_0^1 d\bar{x} \Sigma^{(0)}(x; \bar{x}) G(\bar{x}; x') = R[G(x; x') - \bar{G}(x')], \quad (4.10)$$

where

$$\bar{G}(x') \doteq \int_0^1 d\bar{x} G(\bar{x}; x').$$

The solution, which we shall call $G^{(1)}$, of the resulting equation

$$([G^{(0)}]^{-1} + \Sigma^{(0)})G^{(1)} = \mathbf{1}$$

is

$$G^{(1)}(x; x') = G_{<}^{(1)}(x; x')H(x' - x) + (x \leftrightarrow x'),$$

where

$$G_{<}^{(1)}(x; x') = 2 \left(\frac{\sinh(\frac{1}{2}R(1-x')) \sinh(\frac{1}{2}Rx)}{\sinh(\frac{1}{2}R)} \right) \cosh(\frac{1}{2}R(x-x')). \quad (4.11)$$

(Note that this reduces correctly to $G^{(0)}$ as $R \rightarrow 0$.) One has

$$\bar{G}^{(1)}(x') = \frac{\sinh(\frac{1}{2}Rx') \sinh(\frac{1}{2}R(1-x'))}{\sinh(\frac{1}{2}R)},$$

so, if one employs a hyperbolic identity, Eq. (4.11) can be written alternatively as

$$G_{<}(x; x') = \bar{G}^{(1)}(x') \left(1 + \frac{\sinh(R(x - \frac{1}{2}x'))}{\sinh(\frac{1}{2}Rx')} \right).$$

As $x \rightarrow x'$, $G_{<}$ rises from 0 to twice $\bar{G}^{(1)}$. The maximum of $\bar{G}^{(1)}$ occurs at $x' = 1/2$ and is $\tanh(\frac{1}{4}R)/2$ (which, of course, approaches $1/2$ as $R \rightarrow \infty$).

Although the equation for $G^{(1)}$ is valid only for small R , its behavior for large R is significant. Unlike $G^{(0)}$, which is unbounded as $R \rightarrow \infty$ and has no boundary layer behavior, $G^{(1)}$ has a finite limit,

$$\lim_{R \rightarrow \infty} G^{(1)} = 1,$$

and does have boundary layers for large R . This change in qualitative behavior occurs when R is so large that advective effects become important, namely for $R \gtrsim 4$ or 5. The renormalization has introduced a self-regulatory term which competes with $[G^{(0)}]^{-1}$. This feature will persist in more complete renormalizations.

A proper description for the large R regime must be fully renormalized, so we turn to the direct-interaction approximation. Although this must be solved numerically, that procedure is straightforward, at least for moderate R . [See Appendix D.] Typical solutions are shown in Figs. 10 through 14. In Fig. 10 the direct-interaction approximation for G is compared to $G^{(1)}$ for $R = 5$ and $x' = 0.33$; Fig. 11 provides the same comparison for $R = 20$. In Fig. 12 we compare G to $G^{(0)}$ for selected x' and for $R = 5$; in Fig. 13 the same comparison is made for $R = 20$. Finally, in Fig. 14 we show $G(x; x')$ for various x' at $R = 20$.

4.4 Solution for renormalized flux

Equations (4.4) and (4.5) can be combined to find a single equation for the flux. The result, which can be written somewhat schematically in the form

$$\left[1 + R^{-1} \left(-R^{-1} \frac{\partial^2}{\partial x^2} + 2\Sigma \right) \right] \Gamma(x) = \bar{\Gamma} + R^{-1}, \quad (4.12)$$

is very similar to Eq. (3.11). Indeed, the renormalization has replaced the inverse of the unperturbed Green's function $G^{(0)} = -R^{-1} \partial^2 / \partial x^2$ by

$$[G^{(0)}]^{-1} \rightarrow [G^{(0)}]^{-1} + 2\Sigma \equiv R^{-1} \mathbf{M}^{-1}.$$

The general form (3.14) of the solution still holds. Since G is known, so is Σ , and Eq. (3.12) can be treated as a linear system which can be solved numerically. The results are presented in Figs. 8 and 9. We see that except possibly at very large R the direct-interaction

approximation is somewhat more accurate than the basic bound; however, its prediction is actually lower than the true result.

In a sense, it is remarkable that the basic bound is as good as it is. The direct-interaction approximation includes substantially more complicated interactions; in particular, it describes approximately the point-to-point effects of triplet correlations, which are not considered in the basic optimum theory. What we learn is that the conservative property of the nonlinear transfer term is a very powerful constraint. The triplet correlations determine the detailed distribution of energy among the various spatial positions and scales (Fourier components, in a homogeneous description), and the precise nature of that distribution does, of course, affect the numerical value of the flux. However, because these effects cancel when averaged across the layer, the effects of the triplet correlations, or the transfer term, are rather subtle relative to the fundamental energy balance between global production and global dissipation described by the basic optimum theory.

5. TIME-DEPENDENT CONSTRAINTS AND THE CASE OF FINITE KUBO NUMBER

As we have remarked several times, the principal physical deficiency of the method as described so far is its inability to take account of the decorrelation processes described by a finite Kubo number, a measure of the autocorrelation time of the advecting field. Not only is the kinetic quasilinear scaling thus precluded, so are most effects of propagating waves or, in a kinetic description, streaming particles. In a self-consistent description, the missing physics is likely to be particularly significant for dielectric media like plasmas that are rich in collective phenomena.

Particle streaming, dielectric response, and wave propagation are all intrinsically two-time- and two-space-point phenomena. Thus, for example, the dielectric function $\mathcal{D}(\mathbf{k}, \omega)$ [not to be confused with the dissipation term $\mathcal{D}(x)$] is the Fourier transform with respect to $\mathbf{p} \doteq \mathbf{x} - \mathbf{x}'$ and $\tau \doteq t - t'$ of the dielectric operator $\mathcal{D}(\mathbf{x}, t; \mathbf{x}', t') = \mathcal{D}(\mathbf{p}, \tau)$, the last relation being true for stationary, homogeneous turbulence. Variational principles which take these phenomena into account must accordingly consider constraints which depend on two time and, most generally, two space points. There are, of course, an infinite number of such constraints, and we have only begun to explore them. Here, we shall be content to show that one such constraint does introduce the Kubo number in a qualitatively correct way, so that one is able to recover from the bounding theory all of the scaling regimes of the physical solution, described in Fig. 2. We shall again demonstrate the technique for the simplest possible example, namely the generalized reference model, Eq. (2.15), which allows an explicit solution of the Euler equation. However, it will be clear that the method is more general. To the best of our knowledge, this is the first use of time-dependent constraints in the context of the optimum theory.⁶

5.1 Quasilinear theory

In order to motivate the time-dependent variational formalism, and also to make contact with the scaling theory described in the Introduction as well as with the exact solution of the reference model, it is useful to recall the "quasilinear" approximation. Thus, we write Eq. (2.16) in the form

$$\begin{aligned} [G^{(0)}]^{-1} \delta T(x, t) &= -\delta u(t) \frac{\partial}{\partial x} \langle T \rangle - \frac{\partial}{\partial x} (\delta u \delta T - \langle \delta u \delta T \rangle) \\ &\doteq -\delta \mathcal{H}(x, t), \end{aligned} \quad (5.1)$$

where

$$\left(\frac{\partial}{\partial t} - R^{-1} \frac{\partial^2}{\partial x^2} \right) G^{(0)}(x, t; x', t') = \delta(t - t') \delta(x - x'). \quad (5.2)$$

Because the temporal Fourier transform of $G^{(0)}$ is often more useful than the time-dependent function itself (see below), we shall write the solution of Eq. (5.2) in the form

$$G^{(0)}(x, \tau; x') = \int \frac{d\omega}{2\pi} e^{-i\omega\tau} G_{<\omega}^{(0)}(x; x') H(x' - x) + (x - x'),$$

where

$$G_{<\omega}^{(0)}(x; x') = R \left[\frac{\sinh(a_\omega(1-x')) \sinh(a_\omega x)}{a_\omega \sinh a_\omega} \right] \quad (5.3a)$$

and

$$a_\omega \doteq (-i\omega R)^{1/2}. \quad (5.3b)$$

This correctly reduces to Eq. (4.9) in the limit $\omega \rightarrow 0$. The Fourier inversion can be performed by residue theory; after some manipulations, one obtains

$$G^{(0)}(x, \tau; x') = 2H(\tau) \sum_{n=1}^{\infty} \sin(n\pi x) \sin(n\pi x') \exp(-n^2 \pi^2 \tau / R). \quad (5.4)$$

This familiar result could also have been obtained directly from Eq. (5.2) by separation of variables with a Fourier sine series.

The formal solution of Eq. (5.1) is

$$\delta T(x, t) = \int_0^1 d\bar{x} G^{(0)}(x, t; \bar{x}, 0) \delta T(\bar{x}, 0) - \int_0^t d\bar{t} \int_0^1 d\bar{x} G^{(0)}(x, t; \bar{x}, \bar{t}) \delta \mathcal{H}(\bar{x}, \bar{t}).$$

If we make the usual assumption that the advecting velocity field is uncorrelated with the initial concentration fluctuations,

$$\langle \delta u(t) \delta T(0) \rangle = 0.$$

then the stationary advective flux is $\Gamma(x) = \lim_{t \rightarrow \infty} \langle \delta u(t) \delta T(x, t) \rangle$, or

$$\Gamma(x) = - \int_0^\infty d\bar{\tau} \int_0^1 d\bar{x} G^{(0)}(x, \bar{\tau}; \bar{x}) \langle \delta u(t) \delta \mathcal{H}(\bar{x}, t - \bar{\tau}) \rangle. \quad (5.5)$$

Equation (5.5) is exact. In general, of course, it involves the unknown triplet correlation $\langle \delta u(t) \delta u(t - \bar{\tau}) \delta T(t - \bar{\tau}) \rangle$. However, in the limit of either small K or R , this term is small in perturbation theory. When we ignore that term, we arrive at the quasilinear approximation:

$$\Gamma(x) = - \int_0^\infty d\bar{\tau} \left[\int_0^1 d\bar{x} G^{(0)}(x, \bar{\tau}; \bar{x}) U(\bar{\tau}) \right] \frac{\partial}{\partial \bar{x}} \langle T \rangle(\bar{x}) \quad (5.6)$$

$$\approx -D_Q(x) \frac{\partial}{\partial x} \langle T \rangle, \quad (5.7)$$

where

$$D_Q(x) = \int_0^\infty d\bar{\tau} \int_0^1 d\bar{x} G^{(0)}(x, \bar{\tau}; \bar{x}) U(\bar{\tau}). \quad (5.8)$$

For small Kubo number ($K \ll R$, $K \ll 1$), the (Markovian) approximation (5.7), local in x , is justified because only the short-time $G^{(0)}$ is relevant, and that function is localized near $x = \bar{x}$. [Classical diffusion has not had time to act; many n 's are important in Eq. (5.4).] For large K , diffusion does have time to delocalize $G^{(0)}$; one has

$$\int_0^\infty d\bar{\tau} G^{(0)}(\bar{\tau}) U(\bar{\tau}) \approx \int_0^\infty d\bar{\tau} G^{(0)}(\bar{\tau}) = G_{\omega=0}^{(0)},$$

where $G_{\omega=0}^{(0)}(x; \bar{x})$ is given by expression (4.9). However, in this limit ($R \ll K$, $R \ll 1$), the concentration gradient is approximately constant at its laminar value of (-1) , so the $\bar{x}$ integral in Eq. (5.6) acts primarily on $G^{(0)}$ and we again recover Eqs. (5.7) and (5.8).

We can recover both the hydrodynamic and kinetic quasilinear results from the above. In the hydrodynamic regime, $\tau_h < \tau_{ac}$, we may assume $U(\bar{\tau}) \approx U(0) = 1$, so that

$$D_h(x) = \int_0^1 d\bar{x} G_{\omega=0}^{(0)}(x; \bar{x}) = \frac{1}{2} R x (1 - x).$$

The mean advective flux may be obtained by averaging Eq. (5.7) and using the laminar value of the concentration gradient:

$$\begin{aligned} \gamma_h &= \int_0^1 D_h(x) \\ &= \frac{1}{12} R, \end{aligned}$$

which agrees with formula (2.14b). In the kinetic regime, the time dependence of U dominates Eq. (5.8):

$$\begin{aligned} D_Q(x) &= \int_0^\infty d\bar{\tau} \int_0^1 d\bar{x} [H(\bar{\tau})\delta(x - \bar{x})]U(\bar{\tau}) \\ &= \int_0^\infty d\bar{\tau} U(\bar{\tau}) \\ &= K. \end{aligned} \quad (5.9)$$

This formula is strictly valid in the limit $\tau_{ac} \rightarrow 0$, K finite, for all points in the open interval $0 < x < 1$. For the boundary points $x = 0$ and $x = 1$, D_Q vanishes. This discontinuous behavior at the boundaries is discussed further in Appendix E.

The above approximations of Eq. (5.8) may be made more explicit if we assume for δu , in addition to the assumption of stationary and Gaussian, the Markov property. Then Doob's theorem³⁷ assures us that the shape of $U(\tau)$ is exponential; in dimensionless units,

$$U(\tau) = \exp(-|\tau|/K). \quad (5.10)$$

Then expression (5.8) becomes

$$D_Q(x) = \int_0^1 d\bar{x} G_\omega^{(0)}(x; \bar{x})|_{\omega=iK^{-1}}.$$

This result embraces both regimes just described. Referring to Eqs. (5.3), we see explicitly the appearance of the ratio R/K , since $a_{\omega=iK^{-1}} = (R/K)^{1/2}$.

5.2 A time-dependent constraint

It is clear that one must consider two-time correlations in order to introduce the Kubo number into the formalism. This is true both on general principles and also from relations such as $K = \int_0^\infty d\bar{\tau} U(\bar{\tau})$. Exact equations for two-time correlations can be obtained from Eq. (5.1) by multiplying either by $\delta T(x', t')$ or by $\delta u(t')$. Motivated by the derivation of Eq. (5.6), we consider the latter possibility here. Let us define

$$\begin{aligned} \Gamma(x, t; x', t') &\doteq \langle \delta T(x, t) \delta u(x', t') \rangle \\ &= \Gamma(x, \tau). \end{aligned}$$

Then we have

$$\begin{aligned} \frac{\partial}{\partial \tau} \Gamma(x, \tau) - R^{-1} \frac{\partial^2}{\partial x^2} \Gamma(x, \tau) + U(\tau) \frac{\partial}{\partial x} \langle T \rangle(x) \\ = - \frac{\partial}{\partial x} \langle \delta u(t) \delta T(x, t) \delta u(t') \rangle. \end{aligned} \quad (5.11)$$

As before, we circumvent the closure problem by annihilating the triplet term with an integration from 0 to 1, taking account of the boundary conditions on δT . (In principle, it is not necessary to annihilate the triplet correlation; it can be retained in the constraint and determined as part of the solution of the variational problem.³⁸ However, this procedure is likely to be rather complicated in practice.) In describing the result, we are faced with a slight difficulty of notation, since we shall soon introduce an integration over time as well and we wish to use the overline notation for that also. Therefore, we shall adopt the convention that when the time (difference) argument is outside the bar [as in $\bar{\Gamma}(\tau)$], only spatial integration is intended; when it is under the bar [as in $\overline{\Gamma(\tau)}$], time integration is implied as well. We shall also indicate by the barring operation integrations over x' and t' , using τ and t' as the time variables. Integration over t' is redundant since we assume stationarity; however, it is useful formally. Similarly, integration over x' is redundant for the equal-space-point correlations we considered earlier. Thus, if for arbitrary A we write $A(x, t; x', t') \equiv A(x, \tau | x', t')$, we define

$$\bar{A}(\tau) \doteq \int_{-\infty}^{\infty} dt' \int_0^1 d\bar{x} dx' A(\bar{x}, \tau | x', t')$$

and

$$\overline{A(x, \tau | x', t')} \equiv \overline{A(\tau)} \doteq \int_{-\infty}^{\infty} d\bar{\tau} \bar{A}(\bar{\tau}).$$

Then we obtain from Eq. (5.11) the exact constraint

$$C(\tau) \doteq \frac{d}{d\tau} \bar{\Gamma}(\tau) - R^{-1} \overline{\Gamma''}(\tau) - U'(\tau) = 0, \quad (5.12)$$

where we used $\overline{\langle T \rangle'} = -1$. [In the general case $U = U(\rho, \tau)$, we could not have exploited the boundary conditions on $\langle T \rangle$ so simply. Rather, we would have had to eliminate $\langle T \rangle'$ by using relation (2.23), thus introducing a nonlinear term into the constraint. This causes no conceptual difficulty.] Note that in the limit of large R , we have under the boundary condition $\bar{\Gamma}(-\infty) = 0$

$$\bar{\Gamma}(\tau) = \int_{-\infty}^{\tau} d\bar{\tau} U(\bar{\tau}),$$

from which

$$\bar{\Gamma}(0) = \gamma = \int_{-\infty}^0 d\bar{\tau} U(\bar{\tau}) = K,$$

in agreement with Eq. (5.9).

5.3 Variational principle with a time-dependent Lagrange multiplier

From the point of view of the variational formalism, the relation (5.12) is actually an infinity of constraints, one for each value of τ . Formally, these may all be introduced simultaneously by use of a time-dependent Lagrange multiplier $\lambda(\tau)$. We shall again work with the minimum form of the principle. Then, the constrained minimum of the functional (2.29), which we shall here call $\mathcal{R}_0$, subject to Eq. (5.12) is equivalent to the unconstrained minimum of the extended functional

$$\mathcal{R}(\gamma; \{\lambda\}) \doteq \mathcal{R}_0(\gamma) + \int_{-\infty}^{\infty} d\bar{\tau} \lambda(\bar{\tau}) \mathcal{C}(\bar{\tau}),$$

or

$$\mathcal{R}(\gamma; \{\lambda\}) = \mathcal{R}_0(\gamma) + \overline{\lambda(\tau) \mathcal{C}(\tau)}.$$

Functional differentiation of $\mathcal{R}$ with respect to $\lambda(\tau)$ reproduces the constraint (5.12), while functional differentiation with respect to $\delta T(t)$ produces the desired Euler equation, now time-dependent.

In performing the required differentiations, one notes that derivatives of $\mathcal{R}_0$ are just as before, and also uses the result that

$$\frac{\delta \bar{\Gamma}(\tau)}{\delta T(x, t)} = \delta u(t - \tau) P\{u\}.$$

(See Appendix A.) The resulting Euler equation can be written in the form

$$\begin{aligned} 0 = & -R^{-1} \delta T''(x, t) + [R \Delta \Gamma(x) - 1] \delta u(t) \\ & - \frac{1}{2} R^{-1} \gamma \int_{-\infty}^{\infty} d\bar{\tau} \left\{ \dot{\lambda}(\bar{\tau}) \delta u(t - \bar{\tau}) + \lambda(\bar{\tau}) \delta u(t - \bar{\tau}) R^{-1} \delta''(\bar{x} - x) \right\}_0^1. \end{aligned} \quad (5.13)$$

We wish to eliminate the Lagrange multiplier by employing the constraint (5.12). To that end, we multiply Eq. (5.13) by $\delta u(t')$ and ensemble-average:

$$\begin{aligned} 0 = & -R^{-1} \Gamma''(x, \tau) + [R \Delta \Gamma(x) - 1] U(\tau) \\ & - \frac{1}{2} R^{-1} \gamma \int_{-\infty}^{\infty} d\bar{\tau} \left\{ \dot{\lambda}(\bar{\tau}) U(\tau - \bar{\tau}) + \lambda(\bar{\tau}) U(\tau - \bar{\tau}) R^{-1} \delta''(\bar{x} - x) \right\}_0^1. \end{aligned} \quad (5.14)$$

Upon integrating in x from 0 to 1, we find

$$0 = -R^{-1} \bar{\Gamma}''(\tau) - U(\tau) - \frac{1}{2} R^{-1} \gamma (\dot{\lambda} * U)(\tau), \quad (5.15)$$

where the star denotes time convolution. Upon comparing Eq. (5.15) to the constraint, Eq. (5.12), we find that

$$(\dot{\lambda} * U)(\tau) = -\frac{2R}{\gamma} \frac{d}{d\tau} \bar{\Gamma}(\tau). \quad (5.16)$$

In addition to $\dot{\lambda} * U$, Eq. (5.14) requires the quantity $\lambda * U$, which may be obtained by direct integration of Eq. (5.16):

$$(\lambda * U)(\tau) = -2R[\bar{\Gamma}(\tau)/\gamma].$$

When this result is inserted into the last term of Eq. (5.14), we see that the role of that term is to provide the proper singular terms necessary for dealing with the function $[H(x) - H(x-1)]\Gamma(x, \tau)$ on the closed interval $[0, 1]$. If we work on the interior of the interval in the conventional way, these terms may be ignored, and we shall subsequently do so.

Upon eliminating the term $\dot{\lambda} * U$ from Eq. (5.14), we find the desired time-dependent Euler equation:

$$\frac{d}{d\tau} \bar{\Gamma}(\tau) - R^{-1} \Gamma''(x, \tau) + [R\Delta\Gamma(x) - 1]U(\tau) = 0. \quad (5.17)$$

Although this is a kind of diffusion equation, notice in particular that the time-derivative term is independent of x . This suggests that separation of variables may be useful. Write Eq. (5.17) in the form

$$-\Gamma''(x, \tau) = R^2\{[\gamma - \Gamma(x) + R^{-1}]U(\tau) - R^{-1}\bar{\Gamma}(\tau)\}. \quad (5.18)$$

The form

$$\Gamma(x, \tau) = \Gamma(x)\Upsilon(\tau), \quad \Upsilon(0) = 1,$$

will be a solution of Eq. (5.18) if $\Upsilon = U$ and $\dot{\Upsilon} \propto U$. This will be true if $\dot{U}/U = \text{constant}$, which is the Markov hypothesis (5.10). Under this assumption, we arrive at a generalization of Eq. (2.35) appropriate for finite Kubo number:

$$-\Gamma''(x) + R^2\Gamma(x) = R^2\{\gamma[1 - (RK)^{-1}] + R^{-1}\}. \quad (5.19)$$

The solution of Eq. (5.19) may be readily obtained by following the procedure used to solve Eq. (2.35). The resulting flux may be conveniently expressed in the form

$$\gamma^{-1}(R, K) = \gamma_{\infty}^{-1}(R) + \gamma_q^{-1}(K), \quad (5.20)$$

where as before $\gamma_q \doteq K$ and γ_{∞} is just the result (2.40b) for the $K = \infty$ reference model. We see that the improved bound has the desired limits. We have

$$\gamma(R, K) \sim \begin{cases} K & (K \rightarrow 0), \\ \gamma_{\infty}(R) & (K \rightarrow \infty). \end{cases}$$

The crossover between regimes occurs when $\gamma_{\infty}(R) \approx K$. For $R \rightarrow \infty$, we have $\Phi \sim 2/R$, so the crossover occurs when $K \approx 1/2$. For $R \rightarrow 0$, $\Phi \sim 1 - R^2/12$, so the crossover occurs when $K \approx R/12$. This is in agreement with the qualitative behavior represented by Fig. 2.

The form of the result (5.20) is similar to the form of the effective diffusion coefficient in a composite medium, where the smaller coefficient dominates the total flux. Formula (5.20) is graphed in Fig. 15.

When the Markov property does not hold, the solution of Eq. (5.17) is more involved, but still tractable. We begin by formally solving Eq. (5.18) for $\Gamma(x, \tau)$ by using the unperturbed Green's function $G^{(0)}$:

$$\Gamma(x, \tau) = -R^2(G^{(0)} * \Gamma)(x)U(\tau) + R^2[(\gamma + R^{-1})U(\tau) - R^{-1}\dot{\bar{\Gamma}}(\tau)](G^{(0)} * \mathbf{1})(x). \quad (5.21)$$

By integrating this from 0 to 1, we obtain an equation for $\bar{\Gamma}(\tau)$. This can be written in the form

$$\dot{\bar{\Gamma}}(\tau) + \nu \bar{\Gamma}(\tau) = R(\gamma - \langle \Gamma \rangle + R^{-1})U(\tau),$$

where, in terms of the quantity

$$\overline{G^{(0)}} \doteq \int_0^1 dx d\bar{x} G^{(0)}(x; \bar{x}) = \frac{1}{12},$$

we have defined

$$\nu \doteq (R\overline{G^{(0)}})^{-1} = \gamma_h^{-1},$$

and

$$\langle \Gamma \rangle \doteq \frac{\int_0^1 dx d\bar{x} G^{(0)}(x; \bar{x}) \Gamma(\bar{x})}{\overline{G^{(0)}}}.$$

(There should be no confusion between this new usage of angular brackets and the ensemble average.) Thus,

$$\bar{\Gamma}(\tau) = R(\gamma - \langle \Gamma \rangle + R^{-1}) \int_{-\infty}^{\tau} d\bar{\tau} e^{-\nu(\tau-\bar{\tau})} U(\bar{\tau}). \quad (5.22)$$

In order to determine γ , we set $\tau = 0$ in Eq. (5.18). We require $\dot{\bar{\Gamma}}(0)$, which from Eq. (5.22) can be written in the form

$$\dot{\bar{\Gamma}}(0) = R\epsilon(\gamma - \langle \Gamma \rangle + R^{-1}),$$

where

$$\epsilon = 1 - \nu \int_{-\infty}^0 d\bar{\tau} e^{\nu\bar{\tau}} U(\bar{\tau}). \quad (5.23)$$

The quantity ϵ is small in the limit $K\nu \gg 1$ ($\gamma_q \gg \gamma_h$). This can be seen explicitly when the Markov assumption is used, for then Eq. (5.23) simplifies to

$$\epsilon = (1 + \nu K)^{-1} = (1 + \gamma_q/\gamma_h)^{-1} \approx \gamma_h/\gamma_q \ll 1. \quad (5.24)$$

In terms of ϵ , we have

$$-\Gamma''(x) + R^2\Gamma(x) = R^2[(\gamma + R^{-1})(1 - \epsilon) + \epsilon\langle\Gamma\rangle], \quad (5.25)$$

which properly reduces to the equation for the basic bound in the limit $\epsilon \rightarrow 0$. The solution of Eq. (5.25) is

$$\Gamma(x) = [(\gamma + R^{-1})(1 - \epsilon) + \epsilon\langle\Gamma\rangle]\hat{\Gamma}(x; R), \quad (5.26)$$

where $\hat{\Gamma}$ was defined by Eq. (2.37). From Eq. (5.26) we obtain

$$\langle\Gamma\rangle = \frac{(1 - \epsilon)(\gamma + R^{-1})(1 - \langle\Phi\rangle)}{1 - \epsilon(1 - \langle\Phi\rangle)}$$

and then

$$\Gamma(x) = \left(\frac{(1 - \epsilon)(\gamma + R^{-1})}{1 - \epsilon(1 - \langle\Phi\rangle)} \right) \hat{\Gamma}(x; R). \quad (5.27)$$

We can now compute $\gamma = \int_0^1 d\bar{x} \Gamma(\bar{x})$. After some straightforward algebra, one may put the result into the form

$$\gamma^{-1} = \gamma_\infty^{-1} + \gamma_0^{-1}, \quad (5.28)$$

where

$$\gamma_0 \doteq \left(\frac{1 - \epsilon}{\epsilon} \right) \left(\frac{1 - \Phi}{R\langle\Phi\rangle} \right). \quad (5.29)$$

By direct computation we find

$$\begin{aligned} \langle\Phi\rangle &= 6 \int_0^1 dx x(1 - x) \left(\frac{\cosh(R(x - \frac{1}{2}))}{\cosh(\frac{1}{2}R)} \right) \\ &= \nu R^{-1}(1 - \Phi), \end{aligned}$$

so we arrive at the very simple result

$$\gamma_0 = \frac{1 - \epsilon}{\nu\epsilon}.$$

With the Markov assumption, this may be reduced further, using Eq. (5.24), to

$$\gamma_0 \rightarrow \gamma_q \doteq K,$$

in complete agreement with our earlier calculation (5.20).

5.4 Concentration profiles for the case of finite Kubo number

We may now consider the profile shapes which are predicted by the present bound. We shall demonstrate that when the Kubo number is sufficiently small [$K < \gamma_\infty(R)$], the profiles are similar to the purely laminar result, even for R large.

With the aid of formulas (5.27), (5.28), and (5.29), the deviation $\Delta\Gamma \doteq \Gamma(x) - \gamma$ can be written in the form

$$\Delta\Gamma(x) = R^{-1} \left(\frac{\gamma}{\gamma_\infty} \right) \left[1 - \left(\frac{1}{2}R \right) \frac{\cosh(R(x - \frac{1}{2}))}{\sinh(\frac{1}{2}R)} \right]$$

[compare this result to Eq. (2.13)], so from Eq. (2.23) the mean concentration gradient predicted by the bound is

$$\frac{d}{dx} \langle T \rangle(x) = -1 + \mathcal{O}(\gamma/\gamma_\infty).$$

Since for $K < \gamma_\infty$ we have $\gamma \approx K$, we see that in the limit of small K the mean concentration gradient is essentially constant, with a value near the laminar result (-1). One may integrate to find the concentration profile itself; after a few manipulations, the result may be put into the form

$$\langle T \rangle(x) = 1 - x - \left[\frac{\gamma(R, K)}{\gamma_\infty(R)} \right] \left[\frac{\sinh(\frac{1}{2}Rx) \cosh(\frac{1}{2}R(1-x))}{\sinh(\frac{1}{2}R)} - x \right].$$

This result is graphed in Fig. 16 for $R = 50$ and various K .

The importance of this behavior is that the bounding theory now embraces an extra degree of locality, so is not so sensitive to the boundary conditions. This is desirable from the point of view of various practical applications, as we discuss in Sec. 7.

6. APPLICATIONS

In this section we shall discuss the relevance of our general formalism to two generic problems which arise in the theory of plasma turbulence. We are concerned with the formulation and interpretation of the principles, rather than with actual numerical results. The reason for this is that, unfortunately, there is no generally accepted model to use for the advecting fields in either example. This is a common difficulty with passive models. Usually the advecting velocity arises from internal, self-consistent fluctuations, so one is led to consider self-consistent bounds. Although we have already reported some work in this direction,⁹ self-consistency is beyond the scope of the present manuscript.

We shall consider in this section the implications of the basic bound only. The quasi-linear limit is well understood in each of the examples we discuss. The scaling transitions between regimes of small and large K will be just as in our general discussions, and in

the absence of a precise numerical computation the extra complication of time-dependent constraints does not seem worthwhile to pursue here.

In drawing the connection between our general results and results in the literature, there is one logical step, common to both examples below, which requires special discussion. Characteristically, scalings for strong turbulence diffusion coefficients have been quoted in terms of a "typical" wave number $\bar{k}$. As in the primitive mixing length arguments,²⁸ we shall identify $\bar{k}^{-1} \sim L$, the width of our slab. One may ask why one cannot choose L to be arbitrarily large relative to the region in which the turbulence is localized. The answer is that the simple optimum scalings are derived under the assumption of a homogeneous advecting field, and also assume that the same differential equations govern the fluctuations throughout the entire region. If the turbulence is localized in space, an extra length will appear in the correlation function $U(x; x)$ and will find its way into the bounds *via* the solution of the relevant integral equation. [Compare Eq. (3.12b).] If the differential equations themselves predict a characteristic scale shorter than L —for example, a magnetic shear-induced radial eigenmode width—this scale may serve as an autocorrelation length and tend to induce quasilinear scaling. [Note that in the quasilinear limit L cancels in the expression for the diffusion coefficient: $D \sim \bar{u}L\gamma$, $\gamma_q \sim K \sim \tau_{ac}/(L/\bar{u})$, $D_q \sim \bar{u}^2\tau_{ac}$.] In lieu of such effects, there is nothing to prevent wavelengths of order the system size from being excited. Of course, the precise value of the transport coefficient depends on the distribution of energy among the various wave numbers, and that is not necessarily reflected accurately by the basic theory. However, the beauty of the method is that even without such accuracy one predicts a rigorous bound.

6.1 Flux in velocity space

First, we shall consider flux in velocity space in a spatially homogeneous, one-dimensional model with specified electric field spectrum. Dupree studied a very similar model in his original work on strong Vlasov turbulence.¹⁰ Dupree's interest was in self-consistent fields, but we now understand³ that his resonance-broadening approximation is much closer in spirit and content to the passive advection problems than to self-consistent ones. Consider the kinetic equation for the probability distribution of test particles:

$$\frac{\partial}{\partial t} f(x, v, t) + v \frac{\partial f}{\partial x} + A(x, t) \frac{\partial f}{\partial v} + C\{f\} = 0.$$

where

$$A(x, t) \doteq \left(\frac{e}{m} \right) E(x, t)$$

is a prescribed random acceleration and where C is a collision operator (which Dupree omitted in Ref. 10). We envision a region in velocity space of width V , within which the

fluctuations are stochastic. For purposes of illustration, we shall use for C the simple Brownian motion approximation,³⁹ where

$$C\{f\} \approx \frac{\partial}{\partial v} \left(\nu v - D_v \frac{\partial}{\partial v} \right) f \quad (6.1)$$

and where the constants ν and D_v are related by the Einstein relation $D_v = v_i^2 \nu$. (Physically, this approximation describes the diffusion of test ions by a sea of electrons.) Equation (6.1) and subsequent formulas can be made to look particularly simple if we write the distribution as a Maxwellian plus a correction,

$$f = f_M(1 + \chi),$$

and introduce a Dirac notation in velocity space,

$$|a(v)\rangle \doteq f_M a(v)$$

and

$$\langle a(v) | b(v) \rangle \doteq \int_{-\infty}^{\infty} dv a(v) [b(v) f_M(v)].$$

Then Eq. (6.1) becomes

$$C\{f\} \approx \hat{C}|\chi\rangle,$$

where

$$\hat{C}|\chi\rangle \doteq -D_v \frac{\partial}{\partial v} \left| \frac{\partial \chi}{\partial v} \right\rangle. \quad (6.2)$$

[The first term on the right-hand side of Eq. (6.1) arises from Eq. (6.2) by "differentiating the ket."] In a homogeneous steady state, we have

$$\frac{\partial}{\partial v} \langle \delta A \delta f \rangle + \langle C\{f\} \rangle = 0,$$

so the law of flux conservation in velocity space is

$$|\Gamma_{\text{tot}}\rangle = -R^{-1} L_{cl}|\chi\rangle + |\Gamma\rangle,$$

where

$$\begin{aligned} \Gamma(v) &\doteq \langle \delta A \delta \chi \rangle, \\ R &\doteq \alpha V / D_v, \end{aligned}$$

and

$$L_{cl}|\chi\rangle = \left| \frac{\partial \chi}{\partial v} \right\rangle.$$

Here α is the total acceleration due to the wave packet:

$$\alpha \doteq \left(\frac{e}{m} \right) \langle \delta E^2 \rangle^{1/2}.$$

We normalize velocities to V , accelerations to α . The basic variational principle is: *Minimize*

$$\mathcal{R}(\gamma) = \gamma \left(\frac{|\delta \chi'|^2 + R^2 \overline{\Delta \Gamma^2}}{\bar{\Gamma}^2} \right) \quad (6.3)$$

subject to

$$\bar{\Gamma} = \gamma.$$

Because the form of Eq. (6.3) is entirely standard, our previous general discussion of scaling applies with obvious transcriptions of notation. The velocity extent V is analogous to the spatial extent L in our previous discussions. A phase space density difference Δf is assumed to be maintained across V . The advective flux can be written as

$$\bar{\Gamma} = -D_a \langle \Delta f \rangle / V.$$

The basic bound on the anomalous velocity space diffusion coefficient scales in the limit of large R (weak collisions) as

$$D_a \sim \alpha V, \quad (6.4a)$$

or

$$D_a \sim \frac{\Delta v^2}{\Delta t}, \quad (6.4b)$$

where

$$\Delta v \sim V, \quad (6.4c)$$

$$\Delta t \sim V/\alpha. \quad (6.4d)$$

The result (6.4) can be written more physically by introducing the trapping velocity v_{tr} ,

$$v_{tr} \sim \left(\frac{e}{m} \right) \langle \delta \varphi^2 \rangle^{1/2}$$

($\delta E = -\nabla \delta \varphi$), and the trapping frequency ω_{tr} ,

$$\omega_{tr} \doteq \bar{k} v_{tr}$$

where $\bar{k}$ is a wave number characteristic of the specified field spectrum. Then

$$\alpha \sim v_{tr} \omega_{tr}.$$

If we are to have the situation envisioned in the Introduction, where the fluctuations completely fill the region, then we should take V to be the island width in velocity space due to the total wave packet:

$$V \sim v_{tr}.$$

With this choice, we find that

$$D_a \sim v_{tr}^2 \omega_{tr},$$

which is precisely the scaling of Dupree's strong turbulence "diffusion" coefficient.

6.2 Transport in stochastic magnetic fields

One of the principal proposed mechanisms for the observed anomalously large electron heat conduction in tokamaks is fine-scaled stochasticity of the confining magnetic field.^{40,41,8} If field lines wander diffusively in the radial (x) direction, radial transport of test particles and heat can arise from the rapid motion of the particles *along* the stochastic field. We will show here that bounds can be given for the magnitude of that transport.

Following most previous workers, we shall consider here the passive situation where the magnetic field configuration is statistically specified. In general, this is not true; usually, the magnetic fluctuations arise from a self-consistent turbulent state. In that situation, further constraints may arise⁴²⁻⁴⁴ which may reduce the true transport from that of the passive case. In any event, the passive problem is clearly defined, and our work below makes immediate contact to previous work on the true scaling of the passive situation.

In this mechanism, the fundamental transport coefficient is the so-called magnetic diffusion coefficient D_m of the magnetic field lines, defined by

$$D_m \doteq \lim_{z \rightarrow \infty} \frac{d}{dz} \langle \delta x^2 \rangle(z).$$

Here z is the direction along the unperturbed magnetic field, which is assumed to have good magnetic flux (KAM) surfaces, and δx is the radial deviation of a field line from a reference flux surface. Test particle transport coefficients can be constructed from D_m by relating parallel distance z to time t . Various regimes of collisionality are described in detail in Ref. 8. For example, in the collisionless regime one has $z = v_{\parallel} t$, and a velocity-dependent test particle diffusion coefficient emerges:

$$D(v_{\parallel}) = D_m |v_{\parallel}|. \quad (6.5)$$

This result can be averaged over a Maxwellian distribution if one desires.

In fundamental work, Rosenbluth *et al.*⁴⁵ introduced a stochastic Liouville equation from which D_m could be computed in principle; they worked out explicitly the quasilinear approximation. (In this limit, the so-called autocorrelation length⁸ $L_{ac} \rightarrow 0$.) In a series of papers,^{46,8} one of the present authors and his coworkers showed how to extend such an approach to include the description of test particle diffusion coefficients in the presence of collisional and renormalization effects. Here, we shall reconsider the fundamental equation used in Ref. 8 from the point of view of the optimum theory. [The discussion of the notation which follows is not entirely self-contained; we refer the reader to Ref. 8 (especially Appendix A) for full details.] Let $P(\mathbf{x}, v_{\parallel}, t)$ be the probability distribution of electron guiding centers moving in a prescribed magnetic field

$$\mathbf{B} = \mathbf{B}_0 + \delta \mathbf{B},$$

where $\mathbf{B}_0$ is a sheared equilibrium with good flux surfaces and $\delta\mathbf{B}$ is a specified perturbation, small with respect to $\mathbf{B}_0$, which is assumed to destroy the flux surfaces over some region. We work in a sheared slab geometry. Then, expanded around some reference radius $x = 0$, the equilibrium field is approximately

$$\mathbf{B}_0 \approx B \left(\hat{z} + \frac{x}{L_s} \hat{y} \right),$$

where L_s measures the strength of the shear. Also, assuming here that $\delta\mathbf{B}$ was originally created from internal fluctuations, we follow a common approximation and assume that $\delta\mathbf{B}$ is derived from a perturbed vector potential in the parallel direction only:

$$\delta\mathbf{B} = -\hat{\mathbf{n}} \times \nabla \delta A_{\parallel}.$$

Furthermore, generalizing the discussion in Ref. 8, we allow for electrostatic fluctuations which induce random $\mathbf{E} \times \mathbf{B}$ drifts:

$$\delta\mathbf{V}_E = \frac{c}{B} \hat{\mathbf{n}} \times \nabla \delta\varphi.$$

Then the electrons are advected by the velocity

$$\delta\mathbf{u}(\mathbf{x}, v_{\parallel}, t) = \frac{c}{B} \hat{\mathbf{n}} \times \nabla \left(\delta\varphi - \frac{v_{\parallel}}{c} \delta A_{\parallel} \right). \quad (6.6)$$

To define a passive advection problem, we *assume* that $\delta\varphi$ and $\delta A_{\parallel}$ are Gaussian random fields. This is, of course, not generally true. If the fields were originally produced by internal self-consistent fluctuations, then they will have specific, non-Gaussian correlations. Even if the perturbations arise externally, the stochasticity will not necessarily obey the Gaussian hypothesis. Nevertheless, the Gaussian assumption is useful and has been made by many authors. Thus, we are led to the stochastic differential equation

$$0 = \frac{\partial}{\partial t} P(\mathbf{x}, v_{\parallel}, t) + v_{\parallel} \frac{\partial}{\partial \ell} P + \hat{C}(v_{\parallel}) P - D_{\perp} \nabla_{\perp}^2 P + \nabla \cdot (\delta\mathbf{u} P), \quad (6.7)$$

where ℓ is the arc length along the unperturbed field lines:

$$\frac{\partial}{\partial \ell} \doteq \frac{\partial}{\partial z} + \frac{x}{L_s} \frac{\partial}{\partial y}.$$

As we explained in Ref. 8 following the discussions of Stix⁴⁰ and Rechester and Rosenbluth,⁴¹ the perpendicular classical diffusion term in $D_{\perp}$ is required to allow the particles to leave their initial lines; the term in $\hat{C}$ describes collisional diffusion along the lines. We assume that y and z are symmetry directions. As in Ref. 6, we could implement an ensemble average by the spatial integral over y and z . However, such an operation leaves

not only x , but also $v_{\parallel}$ as a remaining variable. Since our concern is with transport of particles in x space, we shall define a bracket operation $\langle \dots \rangle$ by

$$\langle F(\mathbf{x}, v_{\parallel}) \rangle = \langle F \rangle(x) \doteq \int_{-\infty}^{\infty} dv_{\parallel} dy dz F(\mathbf{x}, v_{\parallel}),$$

where F is an arbitrary function. If we introduce a scalar product in velocity space as we did in Sec. 6.1, we can write

$$\langle F \rangle \doteq \langle 1 | F \rangle.$$

Note that, since $\hat{C}$ is number-conserving, one has

$$\langle 1 | \hat{C} = 0.$$

Then, upon averaging Eq. (6.7) by applying $\langle 1 |$, we find a typical statement of continuity for the mean density of test particles:

$$0 = -D_{\perp} \frac{d^2}{dx^2} \langle n \rangle(x) + \frac{d}{dx} \Gamma(x),$$

where

$$\begin{aligned} n(\mathbf{x}, t) &\doteq \int_{-\infty}^{\infty} dv_{\parallel} P(\mathbf{x}, v_{\parallel}, t), \\ \langle n \rangle(x) &= \langle 1 | \chi \rangle, \\ \Gamma(x) &= \hat{\mathbf{x}} \cdot \mathbf{\Gamma}(x), \\ \mathbf{\Gamma}(x) &\doteq \langle \delta P(\mathbf{x}, v_{\parallel}, t) \delta \mathbf{u}(\mathbf{x}, v_{\parallel}, t) \rangle \\ &\equiv \langle \delta \chi | \delta \mathbf{u} \rangle. \end{aligned}$$

As usual, it is useful to introduce dimensionless variables. We shall again call the rms level of the advecting field $\bar{u}$:

$$\begin{aligned} \bar{u} &\doteq \|\delta u_x\| \\ &= \left[\left(\frac{c}{B} \right)^2 \langle \delta E_y^2 \rangle + v_t^2 \left\langle \left(\frac{\delta B_x}{B} \right)^2 \right\rangle \right]^{1/2}, \end{aligned} \quad (6.8)$$

the latter result holding under the assumption that $\delta \varphi$ and $\delta A_{\parallel}$ are uncorrelated (which need not be true if they arise from self-consistent turbulence). It is convenient to normalize perpendicular velocities to $\bar{u}$, but to normalize parallel velocities to the thermal velocity v_t . As before, lengths are scaled to L , the width in x of the region over which the stochasticity assumption is valid; times are scaled to τ_L . Then Eq. (6.7) becomes

$$0 = \frac{\partial}{\partial t} P(\mathbf{x}, v_{\parallel}, t) + v_{\parallel} \frac{\partial}{\partial \ell} P + \hat{v} \hat{C}(v_{\parallel}) P - R^{-1} \nabla_{\perp}^2 P + \nabla \cdot (\delta \mathbf{u} P), \quad (6.9)$$

where $\dot{\nu} \doteq \nu \tau_L$, and the continuity relation is

$$0 = -R^{-1} \frac{d^2}{dx^2} \langle n \rangle(x) + \frac{d}{dx} \Gamma(x),$$

the integral of which is again just Eq. (2.10b).

The fluctuations obey

$$0 = \left(\frac{\partial}{\partial t} + v_{\parallel} \frac{\partial}{\partial \ell} + \dot{\nu} \hat{C} - R^{-1} \nabla_{\perp}^2 \right) \delta P + \delta \mathbf{u} \cdot \nabla \langle P \rangle + \nabla \cdot (\delta \mathbf{u} \delta P - \langle \delta \mathbf{u} \delta P \rangle). \quad (6.10)$$

Upon multiplying Eq. (6.10) by δP and averaging, we obtain

$$0 = \dot{\nu} \langle \delta P \hat{C} \delta P \rangle - R^{-1} \langle \delta P \nabla_{\perp}^2 \delta P \rangle + \Gamma \frac{d}{dx} \langle n \rangle + \frac{d}{dx} \langle \frac{1}{2} \delta u_x \delta P^2 \rangle;$$

upon integrating this over the layer and eliminating the mean gradient, we obtain the constraint

$$\bar{\Gamma} = \overline{\dot{\nu} \delta P \hat{C} \delta P} + R^{-1} \overline{|\nabla_{\perp} \delta P|^2} + R \overline{\Delta \Gamma^2}.$$

The basic variational principal is: *Minimize*

$$\mathcal{R}\{\gamma\} = \gamma \left(\frac{\overline{R \dot{\nu} \delta P \hat{C} \delta P} + \overline{|\nabla_{\perp} \delta P|^2} + R^2 \overline{\Delta \Gamma^2}}{\bar{\Gamma}^2} \right) \quad (6.11)$$

subject to $\bar{\Gamma} = \gamma$.

Equation (6.11) is very similar to the variational principle (2.30) for the reference model, except for one extra term which describes the effects of collisions. Thus, the Euler equation is very similar to Eq. (2.34) [see also Eq. (3.9)]:

$$\left(-\frac{\partial^2}{\partial x^2} + R \dot{\nu} \hat{C} \right) |\delta \chi\rangle = -R^2 |\delta u\rangle [\Gamma(x) - (\gamma + R^{-1})]. \quad (6.12)$$

In general, solution of Eq. (6.12) is somewhat complicated because of the collision operator and the dependence (6.6) of $|\delta u\rangle$ on $v_{\parallel}$. To illustrate the physical content of Eq. (6.12), we shall consider two limits which are easily solvable. In the first (and most relevant physically), we neglect collisions entirely: $\dot{\nu} = 0$. Then we have exactly the situation described in Sec. 3.1. Furthermore, let us ignore the dependence of δu on x . This is a conceivable limit for the magnetic fluctuations; see Ref. 8. It is less realistic for $\mathbf{E} \times \mathbf{B}$ turbulence, for that, we should properly employ the equations (3.12)–(3.14). However, this detail will affect numerical coefficients, not the gross scaling. Here, we are concerned more with the interpretation of the terms. Thus, we proceed by ignoring x dependence. Then, just as in Sec. 2.3, we can form an equation for the flux by multiplying Eq. (6.12)

by $\langle \delta u \rangle$. Since we have normalized velocities according to Eq. (6.8), the resulting equation is identical to Eq. (2.35), and we are led again to the result (2.40). In the important limit $R \rightarrow \infty$, the resulting (strong turbulence) scaling for the bound,

$$D \sim \bar{u}L,$$

can be written in the form

$$D \sim (v_E^2 + v_t^2 \langle \delta b^2 \rangle)^{1/2} L, \quad (6.13)$$

where v_E is the rms level of the x component of the $\mathbf{E} \times \mathbf{B}$ velocity and $\delta b \doteq \delta B_z/B$. In the limit $\delta b \rightarrow 0$, Eq. (6.13) reduces to

$$D \sim v_E L,$$

which is another strong turbulence scaling of Dupree.⁴⁷ (Dupree writes $D \sim v_E \bar{k}^{-1}$, where $\bar{k}$ is a typical wave number; see the discussion at the beginning of this section.) In the limit $\delta \varphi \rightarrow 0$, we find instead

$$D \sim \langle \delta b^2 \rangle^{1/2} L v_t.$$

This is in agreement with the result (6.5) when the strong turbulence scaling

$$D_m \sim \langle \delta b^2 \rangle^{1/2} L \quad (6.14)$$

is used for the magnetic diffusion coefficient. This scaling was first given by Kadomtsev and Pogutse⁴⁸ (again with the inverse of a characteristic wave number replacing L), and is also briefly described in Ref. 8.

In the second limit, we retain collisions but ignore electrostatic fluctuations—precisely the approximation discussed in Ref. 8. Now, the right-hand side of Eq. (6.12) is proportional to $v_{||}$. We obtain an explicitly solvable model if we again use for $\hat{C}$ the operator (6.1), for which $|v_{||}\rangle$ is an eigenfunction with unit eigenvalue:

$$\hat{C}|v_{||}\rangle = |v_{||}\rangle.$$

Let us also assume for simplicity⁸ that

$$\delta \mathbf{B}(\mathbf{x}) \approx \hat{\mathbf{x}} \delta b(y, z),$$

a form which respects $\nabla \cdot \mathbf{B} = 0$ in slab geometry. The solution of Eq. (6.12) then has the form

$$|\delta \chi\rangle = \psi(x) \delta b(y, z) |v_{||}\rangle = \psi(x) |\delta u\rangle, \quad (6.15)$$

where ψ is unknown. Now note that

$$\Gamma(x) = \langle \delta u | \delta \chi \rangle.$$

Upon using Eq. (6.15) and recalling the normalization (6.8), we identify $\psi(x)$ with the advective flux itself:

$$\Gamma(x) = \psi(x).$$

Thus, we are led to the Euler equation

$$-\Gamma''(x) + R_\nu^2 \Gamma(x) = R^2(\gamma + R^{-1}), \quad (6.16)$$

where

$$R_\nu^2 \doteq R^2 \left(1 + \frac{\hat{\nu}}{R} \right). \quad (6.17)$$

Equation (6.16) is very similar to Eq. (2.35). Its solution is

$$\Gamma(x) = \left(\frac{R^2}{R_\nu^2} \right) (\gamma + R^{-1}) \hat{\Gamma}(x; R_\nu), \quad (6.18)$$

which should be compared with Eq. (2.37). Not surprisingly, the collisional effects have modified the structure of the boundary layers. We shall give a physical interpretation after we compute the solution for the bound $\gamma(R; \hat{\nu})$.

The solution of Eq. (6.18) for $\gamma = \int_0^1 d\bar{x} \Gamma(\bar{x})$ can be written in the form

$$\gamma = R^{-1} \left(-1 + \frac{\lambda^2}{\lambda^2 - 1 + \Phi(R\lambda)} \right), \quad (6.19)$$

where

$$\lambda^2 \doteq (R_\nu/R)^2 = 1 + \hat{\nu}/R \quad (6.20)$$

and $\Phi(z)$ was defined by Eq. (2.39a). Equation (6.19) properly reduces to Eq. (2.40) in the limit $\lambda \rightarrow 1$ ($\hat{\nu} \rightarrow 0$). For later use, it will be convenient to write Eq. (6.19) in the form

$$\gamma = R^{-1} \left(\frac{1 - \Phi(R\lambda)}{\hat{\nu}/R + \Phi(R\lambda)} \right). \quad (6.21)$$

For fixed R , let us consider maximizing $\gamma(R; \hat{\nu})$ with respect to $\hat{\nu}$ (or λ). The derivative of γ with respect to λ is proportional to the expression

$$-2 + 3\Phi(z) - \text{sech}^2\left(\frac{1}{2}z\right) \leq 0,$$

where $z \doteq R\lambda$. This vanishes only at $z = 0$, which is not allowed for nonzero R since $\lambda \geq 1$. Thus, for fixed R , the most pessimistic bound occurs for the collisionless limit $\hat{\nu} = 0$.

Various scaling regimes emerge by inspection of Eq. (6.21). It is convenient to use $R\lambda$ initially as the asymptotic parameter, then to relate λ to $\hat{\nu}$. For $R\lambda \ll 1$, one has $\Phi = 1 + \mathcal{O}((R\lambda)^2)$, so

$$\gamma \sim R^{-1} \frac{(R\lambda)^2}{1 + \hat{\nu}/R} \sim R = \gamma_h.$$

[We noted Eq. (6.20).] For sufficiently small $\hat{\nu}$, the criterion $R\lambda < 1$ is equivalent to $R < 1$. For large $\hat{\nu}$, it is equivalent to $\hat{\nu}R < 1$.

For $R\lambda > 1$, one has $\Phi = \mathcal{O}((R\lambda)^{-1})$ and

$$\begin{aligned}\gamma &\sim R^{-1} \left(\frac{1}{\hat{\nu}/R + 1/R\lambda} \right) \\ &= \frac{1}{\hat{\nu} + \lambda^{-1}}.\end{aligned}$$

Two scaling regimes are separated by $\hat{\nu}\lambda \sim 1$. Since $R\lambda > 1$ and since $\lambda \geq 1$, this boundary has $\hat{\nu}/R < 1$, whence from (6.20) $\lambda \sim 1$ and then $\hat{\nu} \sim 1$. For $\hat{\nu}\lambda < 1$,

$$\gamma \sim \lambda \sim 1 = \gamma_s;$$

for $\hat{\nu}\lambda > 1$,

$$\gamma \sim \hat{\nu}^{-1} \doteq \gamma_f.$$

This latter scaling has appeared for the first time in this work, and is unique to the collisional regime. The subscript “f” stands for “fluid,” a notation which was introduced in Ref. 8.

Let us consider the dimensional consequences of the bounds γ_s , γ_h , and γ_f , recalling the relationship (1.6) and noting that, since we are now ignoring $\delta\varphi$, $\bar{u} \sim \langle \delta b^2 \rangle^{1/2} v_t$. In terms of particle diffusion coefficients, we have first

$$\begin{aligned}D_s &\sim \bar{u}L \\ &\sim \langle \delta b^2 \rangle^{1/2} L v_t \\ &\sim D_m v_t,\end{aligned}$$

where D_m is defined by Eq. (6.14). In the nomenclature of Ref. 8, this is the well-known result for the collisionless regime, where the basic optimum theory has produced for the bound the strong turbulence version (6.14) of the magnetic diffusion coefficient.

The hydrodynamic diffusion coefficient is

$$\begin{aligned}D_h &\sim (\bar{u}L)\gamma_h \\ &\sim \bar{u}^2 \tau_h \\ &\sim \langle \delta b^2 \rangle v_t^2 \tau_h.\end{aligned}$$

This result was called the double-streaming coefficient in Ref. 8.

Finally, the flux γ_f corresponds to

$$\begin{aligned} D_f &\sim (\bar{u}L)\gamma_f \\ &\sim \bar{u}^2/\nu \\ &\sim \langle \delta b^2 \rangle D_{\parallel}, \end{aligned}$$

where

$$D_{\parallel} \doteq v_t^2/\nu$$

is the classical parallel diffusion coefficient. The interpretation of D_f has been described in detail in Ref. 8 and in previous work.⁴⁹ It describes a radial diffusion process caused by the slow collisional diffusion of particles *along* the perturbed field lines, which have a small, stochastic radial component.

The scaling situation for the bounds in the presence of collisions is presented in Fig. 17. The structure of this figure and the behavior of the bounds are very similar to those of Fig. 2 if one replaces $\hat{\nu}^{-1}$ by the Kubo number K . There is a very important distinction, however. Here, we are describing the basic bounds. All of our scalings are determined by dynamics explicitly described by the equations of motion; no Kubo number appears. In the true situation for stochastic magnetic fields one must also introduce,⁸ in addition to the parameters $\hat{\nu}$ and R , an autocorrelation length L_{ac} , a characteristic of the imposed magnetic perturbations which defines a true Kubo number. Thus, as is very clear from Table 1 of Ref. 8, the true parameter space is three-dimensional. Nevertheless, the bounds we obtain are valid for all regimes. Furthermore, we could explicitly introduce the quasi-linear scaling by considering two-time constraints, which here would involve the dynamics of particle streaming along the unperturbed field lines.

Now we shall discuss the boundary layer behavior of the result (6.18), which is rather subtle and interesting. In general, boundary layers of width $\Delta \sim R_\nu^{-1}$ exist for $R_\nu > 1$. For $\hat{\nu}/R < 1$, this is the familiar behavior of the reference model,

$$\Delta_{cl} \sim R^{-1} \sim D_{\perp}.$$

For $\hat{\nu}/R > 1$, however, the width changes to

$$\Delta_f \sim (\hat{\nu}R)^{-1/2} < \Delta_{cl}. \quad (6.22)$$

The presence of such a narrow boundary layer is perhaps counter-intuitive, but can be explained in terms of the concepts introduced in Ref. 8. First, observe that in our model, admittedly very idealized, the field lines are assumed to be uniformly stochastic all the way to the boundaries. Particles will flow very rapidly along those lines; if the hydrodynamic time is long enough, that flow will wash out the classical boundary layer. However, the constraint that the advective flux vanish at the boundaries means that flux sufficiently near the walls must be classical, so that some sort of boundary layer is still expected. To estimate its width, one must be precise about the flow along the lines. Recall from Ref. 8 the

interesting process of *double diffusion*: For sufficiently long times, particles do not stream with constant velocity, but rather collisionally diffuse along the lines, which are themselves diffusing in x . The resulting radial dispersion, which is slower than diffusive, gives rise to a time-dependent diffusion function $D(t) \sim D_m v_t / (\nu t)^{1/2}$ which must be evaluated at some characteristic decorrelation time. Because the flux must be classical through the boundaries, the classical time τ_h is appropriate. The resulting diffusion coefficient was called the Kadomtsev-Pogutse coefficient in Ref. 8:

$$\begin{aligned} D(\tau_h) &\doteq D_{KP} = D_m v_t / (\nu \tau_h)^{1/2} \\ &= \bar{u} L / (\nu R)^{1/2}. \end{aligned}$$

This diffusion coefficient must carry the doubly diffusing particles, moving radially with velocity $\bar{u}$, through the boundary layer. By continuity,

$$D_{KP} / \Delta r \sim \bar{u},$$

which leads to precisely the result (6.22).

7. DISCUSSION AND CONCLUSIONS

We have shown that the optimum theory of Howard, Busse, and others can be applied to problems of passive advection as well as to self-consistent problems. We illustrated the basic theory, which uses only the steady-state energy balance as a constraint, by studying an exactly soluble case (one dimension, infinite Kubo number); the bound on the flux through the slab compared favorably to the exact result and to the prediction of the much more complicated direct-interaction approximation. By liberal use of Green's functions, we showed how to generalize the variational principle to include various complicated situations, such as higher dimensionality or unusual boundary conditions, which could arise in practice. We extended the formalism to include two-time constraints, and showed that we could derive a bound which had the physical scalings in all regimes of Reynolds and Kubo number. We formulated the basic principle for two situations of interest in plasma physics: transport in velocity space, and transport in space across a stochastic magnetic field. In the latter calculation, contact was made to earlier work in which the true scaling situation was studied in detail.

Although we have cited various practical situations in which the passive assumption is justifiable or has been used, we believe that the principal feature of this work is its pedagogical content. It is useful to have explicit solutions to guide further work. Whatever failings the passive formalism contains will almost certainly appear as well in a self-consistent treatment. Thus, it is comforting to know that the simplest strong turbulence bound is likely to be within about one (rather than many more than one) order of magnitude of the correct answer. It is important to understand the rudiments of a formalism whereby two-time constraints can be taken into account; we expect such a formalism to provide

substantial improvements, both qualitative and quantitative, on the bounds in situations in which particle streaming, wave propagation, or dielectric response is important.

The optimum theory has several desirable philosophical features, in addition to the most important one that it predicts a rigorous bound from above. For example, historically the popular closures in plasma physics were oriented first toward two-time correlations¹⁰; only later were the effects of one-time balances added¹⁴ (in a rather complicated way). In contrast, the basic optimum bound emerges from the simplest aspects of one-time theory; if one desires, it can then be refined by adding more complicated two-time constraints. Related to this is the fact that bounding results for the flux, the quantity of most immediate physical interest, emerge without the necessity of deriving detailed dynamical predictions for fluctuation spectra. The theory uses global balances in space to achieve its predictions and is thus well-suited for intrinsically inhomogeneous situations, such as typical plasma confinement geometries with magnetic shear. Since it is variational, efficient numerical methods are available for its solutions.

When the theory is extended to include self-consistency, several new features emerge. First, because the velocity field now responds self-consistently, the Euler-Lagrange equations become nonlinear and intrinsically more complicated than those of the passive problems. The boundary layer structure is accordingly more involved; nested boundary layers may appear.⁶ The solutions of the Euler-Lagrange equations exhibit bifurcations⁵⁰ into various advective states qualitatively consistent with those experimentally observed in the transition to turbulence. (Detailed agreement should not be expected, especially in the time-independent basic theory.) In particular, there is a critical parameter below which the advective transport vanishes identically. This behavior cannot occur in the passive problems since the variational equations are linear. There, the threshold for stochastic behavior occurs at zero amplitude of the advecting field, and there is advective transport at all values of R and K (although for some parameters it is dominated by classical effects).

An important general application is to the theory of anomalous transport of magnetically confined plasma in the tokamak geometry. We shall not attempt any such calculation here. However, we may ask to what extent it is likely that methods such as these (extended to include self-consistency) may be usefully applied to that very practical problem. The principal qualitative argument which can be raised against such application is concerned with the rigid boundary conditions we have used in formulating the variational principles. These conditions are appropriate when the system is bounded by physical walls. The tokamak is so bounded, but it is not usual (because of extreme complexity) to consider the entire cross-section of the tokamak within the context of one unified model. Instead, various regimes of rather different physical behavior have been experimentally and, to some extent, theoretically identified: (1) the center, interior to the so-called inversion radius r_1 where the "safety factor" q is equal to 1, which typically undergoes relaxation oscillations of temperature ("sawteeth") related to internal MHD instability and the redistribution of magnetic flux; (2) the "good confinement region" between $q = 1$ and some outer radius r_2

often identified with $q = 2$; (3) an edge region, cooler than regions (1) and (2). Microinstabilities are believed to be responsible for the anomalous flux in regions (2) and (3). Although the character of the fluctuations changes as a function of radius, that transition should be gradual. If one considers the thought experiment of excising for analysis a slab of plasma between radii r_a and r_b such that $r_1 < r_a < r_b < r_2$, it is difficult to find theoretical support for the notion that either the density, temperature, or potential fluctuations vanish identically at r_a and r_b . Related to this difficulty is the experimental fact that profiles extremely far from laminar, such as may be suggested by the theory of the basic bound, are not usually observed. (However, rather flat temperature profiles, reminiscent of strong convection, have been observed in the edge region of the Tokamak Fusion Test Reactor.⁵¹) Thus, current approaches to the tokamak transport problem, including both gyrokinetic particle simulations⁵² and closure approximations, usually assume constant gradients of density and temperature and apply periodic boundary conditions in x to the layer of plasma under consideration, whose width L is assumed to be much smaller than the macroscopic scale lengths. However, one is still faced with the problem of determining L . In the absence of magnetic shear, all one really knows is that L should be much greater than the "sound radius" ρ_s . When shear-free simulations are performed with L of order the experimentally determined radial correlation length, typically the longest wavelength modes allowed ($k_{\min} = 2\pi/L$) are excited.⁵³ This suggests either that one should really be working in a box of macroscopic size, with realistic boundary conditions, or, more likely, that shear provides an important localizing effect. In either event, the present formalism seems just as suitable as the alternative approaches. In particular, if the physics actually contains short correlation lengths and times, the additional effects included in the two-time theory substantially ameliorate the tendency toward profile flattening predicted by the basic bound. Although it remains true that even for small Kubo number there is a vestige of boundary layer effects very close to the walls, these effects do not contribute importantly to the flux.

Nevertheless, one might ask why one does not consider the inverse problem: Instead of specifying the concentration at the walls, specify instead the total flux through the slab and attempt to determine a bound on the concentration difference. The reason is that this problem is ill-defined; more statistical moments than the flux must be specified in order to pin down the concentration.

In this paper we have not discussed the effects of sources (in particular, nonconservative terms proportional to some power of the concentration field itself). In some cases it is possible to build a model in which the sources are placed outside of the region of interest. For example, one might approximate the Ohmic heating of a tokamak as concentrated at the center, since the temperature profile is peaked there. In general, however, sources within the region may be physically important. For certain classes of sources, there appears to be no difficulty in principle with extending the formalism to include them. However, because the most general source functions which can be embraced by the formalism are unknown at this time, we shall leave the treatment of sources to future work.

So far, we have spoken as though the turbulence in question were fully developed. It is not entirely clear that this assumption is justifiable for typical classes of tokamak microturbulence. Even if it is not, it would still be a legitimate theoretical exercise to study the fully developed case, since this approximation has been made, usually without comment, in almost all theoretical treatment of plasma microturbulence, for example in the versions of the clump theory represented by Ref. 14. However, an important feature of the present formalism is that it is specifically *not* restricted to the fully developed limit. If an averaging procedure can be found such that the energy is stationary, then the bounds are rigorous properties of the given differential equations, whether or not they are turbulent. The bounding theory produces valid results even when only a few modes are excited.

An additional concern is whether the theory, represented by the Euler-Lagrange equations, is computable for typical practical applications. For the case of the basic passive bound, the answer seems clearly to be "yes," because the equations are linear. (See Sec. 3.1.) For the extension to self-consistency, we are also cautiously optimistic, in part because of our experience with work not presented here.⁹ To obtain the basic bound, Euler equations of elliptic type must be solved. Efficient methods are available for such solution, and various applications have been made in the arena of fluid mechanics.⁶ We have constructed and are testing a computer code^{5d} intended to solve a variety of such problems. The modifications which must be introduced in order to embrace the theory of two-time constraints have not been fully considered; this entire area is a subject of active research. It is not clear that the computational problem of the two-time optimum theory will be substantially simpler than that of the direct-interaction approximation, which with the advent of supercomputers is becoming more tractable, at least for certain plasma problems described by fluid approximations. For either of these approaches, much more work is required.

In conclusion, the variational method represents an alternative approach to the determination of transport coefficients. Its rigor is appealing, and the method has been applied successfully in various problems of fluid dynamics. It remains to be seen just how useful it will be for more complicated problems involving mixtures of waves and eddies, such as occur in the theory of plasma confinement. Advances are being made on the competing theories as well, including the theory of particle simulation,⁵² numerical solution of the direct-interaction approximation,^{55,11} and Kraichnan's decimation scheme,⁵⁶ which unifies a number of different approaches. Ultimately, it will be only by comparing the predictions of all of these approaches that a truly complete and believable theory of turbulent transport will emerge.

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APPENDIX A. THE MEANING OF THE FUNCTIONAL DERIVATIVE

In the original self-consistent applications, what we call here the ensemble average $\langle \dots \rangle$ was taken to be the spatial integral over the homogeneous directions⁶:

$$\langle A(\mathbf{x}, t) \rangle = \langle A \rangle(\mathbf{x}, t) \doteq \int dy dz A(\mathbf{x}, t).$$

Therefore, the layer integral of an ensemble average was the complete spatial integral over the volume,

$$\bar{A} \doteq \int_0^1 d\mathbf{x} \langle A(\mathbf{x}, t) \rangle = \int d\mathbf{x} A(\mathbf{x}, t),$$

and functional derivatives had the meaning standard in the multidimensional calculus of variations.³¹ In particular, the fundamental derivative was

$$\frac{\delta T(\mathbf{x})}{\delta T(\mathbf{x}')} = \delta(\mathbf{x} - \mathbf{x}')$$

and similarly for a second field $u(\mathbf{x})$. Thus, if $f(T(\mathbf{x}), u(\mathbf{x}))$ was a polynomial function of the two fields T and u , and $F\{T, u\} \doteq \bar{f}$, then

$$\begin{aligned} \frac{\delta F\{T, u\}}{\delta T(\mathbf{x})} &= \int d\bar{\mathbf{x}} \frac{\delta}{\delta T(\mathbf{x})} f(T(\bar{\mathbf{x}}), u(\bar{\mathbf{x}})) \\ &= \int d\bar{\mathbf{x}} \frac{\partial f(T, u)}{\partial T} \Big|_{\bar{\mathbf{x}}} \delta(\bar{\mathbf{x}} - \mathbf{x}) \\ &= \frac{\partial f(T, u)}{\partial T} \Big|_{\mathbf{x}}. \end{aligned}$$

In the present work, we use instead of the spatial integral a more general ensemble average, and it is important to understand exactly what the derivative means in this

situation. In this passive calculation, the field $u(\mathbf{x})$ is not to be varied; rather, it describes a particular point in the function space of all fields. The dynamical variable T depends parametrically on the position in space, and functionally on u [that is, it depends on the values of $u(\mathbf{x})$ at all space points $\mathbf{x}$]:

$$T(\mathbf{x}) \equiv T(\mathbf{x}; \{u\}).$$

Consider

$$\begin{aligned} F\{T\} &\doteq \int_0^1 d\mathbf{x} \langle f(T(\mathbf{x}; \{u\}), u(\mathbf{x})) \rangle \\ &= \int_0^1 d\bar{\mathbf{x}} \int D[\bar{u}] P\{\bar{u}\} f(T(\bar{\mathbf{x}}; \{\bar{u}\}), u(\bar{\mathbf{x}})). \end{aligned} \quad (\text{A.1})$$

Because the statistics are assumed to be homogeneous in the y and z directions (which we take here to have unit extent), we may replace $\int d\bar{\mathbf{x}}$ by $\int d\bar{x}$ without changing the value of Eq. (A.1). Then the functional derivative with respect to T at a particular position $\mathbf{x}$ and for a particular realization u is

$$\begin{aligned} \frac{\delta F\{T\}}{\delta T(\mathbf{x}; \{u\})} &= \int_0^1 d\bar{x} \int D[\bar{u}] P\{\bar{u}\} \frac{\partial}{\partial T} f(T, u)|_{\bar{\mathbf{x}}, \bar{u}(\bar{\mathbf{x}})} \delta(\bar{\mathbf{x}} - \mathbf{x}) \delta(\{\bar{u}\} - \{u\}) \\ &= \frac{\partial}{\partial T} f(T(\mathbf{x}; \{u\}), u(\mathbf{x})) P\{u\}. \end{aligned}$$

APPENDIX B. THE MAXIMUM PRINCIPLE AND LAGRANGE MULTIPLIERS

Here we show that the direct, maximum principle leads to the same Euler equation as the more efficient minimum principle. We shall do this for $K = \infty$, but for the general equations introduced in Sec. 3. Thus, we are asked to maximize

$$\bar{\Gamma} + \lambda \left(\bar{\Gamma} - R^{-1} \overline{\delta T \kappa \mathcal{L} \delta T} - R \overline{\Delta \Gamma^2} \right).$$

The Euler equation is

$$\kappa(x) \mathcal{L} \delta T(x) + R^2 u(x) \Delta \Gamma(x) = \frac{1}{2} R u(x) \left(\frac{1 + \lambda}{\lambda} \right). \quad (\text{B.1})$$

In order to determine λ , multiply Eq. (B.1) by δT and bar:

$$\overline{\delta T \kappa \mathcal{L} \delta T} + R^2 \overline{\Delta \Gamma^2} = \frac{1}{2} R \left(\frac{1 + \lambda}{\lambda} \right) \bar{\Gamma}.$$

Upon comparing this equation with the constraint Eq. (3.6), one finds that

$$\frac{1}{2} \left(\frac{1 + \lambda}{\lambda} \right) = 1. \quad (\text{B.2})$$

Upon using this result in Eq. (B.1), one finds an equation identical to Eq. (3.8). Of course, the solution of Eq. (B.2) is $\lambda = 1$, although we do not need this result explicitly.

The determination of the Lagrange multiplier is relatively trivial in the passive problem, although the minimum principle is still preferred for reasons of economy and simplicity. In the self-consistent problems, which sometimes require two Lagrange multipliers, the minimum principle is usually preferred.

APPENDIX C. DERIVATION OF THE DIRECT-INTERACTION APPROXIMATION

The derivation of the direct-interaction approximation for a given stochastic differential equation is by now a reasonably standard procedure. Various techniques are reviewed in Ref. 3, in which many references to Kraichnan's original work are cited. (For stochastic differential equations, see in particular Ref. 7.) The most profound methods are those based on field theory,^{1,57,58} and that work provides, once and for all, a recipe from which, given the equation of motion, the direct-interaction approximation can be written down practically by inspection. One is required only to identify the "bare interaction vertices" and to understand the general structure of the renormalized field equations.³ We have carried out this procedure; the results are equivalent to those of the alternative derivation which follows.

Recipes are dangerous, of course, if one has not studied the original derivations in some detail. The most straightforward method which leads to the desired answer is the iteration-reversion scheme.⁵⁸ This is also a recipe whose justification must be argued separately, but the technique does help to identify the physical significance of the various terms which arise. We shall present the details of this calculation here.

First, we require an equation for the infinitesimal response function G . This function is the statistical mean of the random infinitesimal response function $\tilde{G}$:

$$G(\mathbf{x}, t; \mathbf{x}', t') \doteq \langle \tilde{G}(\mathbf{x}, t; \mathbf{x}', t') \rangle.$$

where

$$\tilde{G}(\mathbf{x}, t; \mathbf{x}', t') \doteq \frac{\delta T(\mathbf{x}, t)}{\delta \hat{\eta}(\mathbf{x}', t')}$$

and where $\hat{\eta}$ is an arbitrary source function added to the fundamental equation of motion Eq. (1.1):

$$\frac{\partial}{\partial t} T(\mathbf{x}, t) + \mathcal{L}T + \nabla \cdot (\mathbf{u}T) = \hat{\eta}(\mathbf{x}, t).$$

We assume that $\mathbf{u}$ is a stationary, centered Gaussian random variable:

$$\begin{aligned}\langle \mathbf{u}(\mathbf{x}, t) \rangle &= 0, \\ \langle \delta \mathbf{u}(\mathbf{x}, t) \delta \mathbf{u}(\mathbf{x}', t') \rangle &= \mathbf{U}(\mathbf{x} - \mathbf{x}', t - t'),\end{aligned}$$

where $\mathbf{U}(\mathbf{p}, \tau)$ is a specified function. The random response function obeys, in an abbreviated notation,

$$\left(\frac{\partial}{\partial t} + \mathcal{L} \right) \tilde{G} - \nabla \cdot (\mathbf{u} \tilde{G}) = \mathbf{I}, \quad (\text{C.1})$$

and the mean response function obeys the average of Eq. (C.1), viz.

$$\left(\frac{\partial}{\partial \tau} + \mathcal{L} \right) G(\mathbf{x}, \tau; \mathbf{x}') + \nabla \cdot \langle \mathbf{u} \tilde{G} \rangle = \delta(\tau) \delta(\mathbf{x} - \mathbf{x}'). \quad (\text{C.2})$$

[In writing Eq. (C.2), we noted that the stationarity of $\mathbf{U}$ implies that G itself is stationary.] The approximation method which leads to the direct-interaction approximation proceeds by introducing an ordering parameter ϵ , assuming that $\mathbf{u}$ is $\mathcal{O}(\epsilon)$, iterating the various quantities in a regular perturbation series through several orders in ϵ , performing statistical averages based on the Gaussian properties of $\mathbf{u}$, then replacing various zeroth-order quantities by their renormalized counterparts. Thus, through first order in $\mathbf{u}$, one has by iteration

$$\tilde{G} \approx G^{(0)} - G^{(0)} \nabla \cdot [\mathbf{u} G^{(0)}], \quad (\text{C.3})$$

where $G^{(0)} \doteq (\partial_\tau + \mathcal{L})^{-1}$. The two-point correlation required for Eq. (C.2) is then approximately (using the notation $1 \doteq \{\mathbf{x}_1, t_1\}$ and the convention of implied integration over repeated indices, and agreeing that gradient operators act all the way to the right)

$$\begin{aligned}\nabla \cdot \langle \mathbf{u}(1) \tilde{G}(1, 1') \rangle &\doteq \hat{\Sigma}(1; \bar{1}) G(\bar{1}, 1') \\ &\approx -\nabla \cdot \langle \mathbf{u}(1) G^{(0)}(1, \bar{1}) \nabla_{\bar{1}} \cdot [\mathbf{u}(\bar{1}) G^{(0)}(\bar{1}, 1')] \rangle \\ &= -\nabla \cdot G^{(0)}(1, \bar{1}) \nabla_{\bar{1}} \cdot \mathbf{U}(1, \bar{1}) G^{(0)}(\bar{1}, 1').\end{aligned} \quad (\text{C.4})$$

(The carat notation reminds us that, because of the gradients, $\hat{\Sigma}$ is here an operator.) The direct-interaction approximation follows from Eq. (C.4) by replacing $G^{(0)}$ by its lowest order reversion from Eq. (C.3), namely

$$G^{(0)} \approx G.$$

Thus, in the direct-interaction approximation

$$\hat{\Sigma}(1; \bar{1}) = -\nabla \cdot [G(1, \bar{1}) \nabla_{\bar{1}} \cdot \mathbf{U}(1, \bar{1})], \quad (\text{C.5})$$

and the final integral (Dyson) equation for the mean response function of the passive advection problem is, after Fourier transformation in the homogeneous directions,

$$\frac{\partial}{\partial \tau} G_{\mathbf{k}}(\mathbf{x}, \tau; \mathbf{x}') + \mathcal{L}_{\mathbf{k}} G_{\mathbf{k}} + \int_0^\tau d\bar{\tau} \int_0^1 d\bar{x} \hat{\Sigma}_{\mathbf{k}}(\mathbf{x}, \bar{\tau}; \bar{\mathbf{x}}) G_{\mathbf{k}}(\bar{\mathbf{x}}, \tau - \bar{\tau}; \mathbf{x}') = \delta(\tau) \delta(\mathbf{x} - \mathbf{x}'),$$

where

$$\hat{\Sigma}_{\mathbf{k}}(x, \tau; x') \doteq -\nabla_{\mathbf{k}} \cdot \sum_{\mathbf{k}'} G_{\mathbf{k}-\mathbf{k}'}(x, \tau; x') \nabla_{\mathbf{k}'} \cdot \mathbf{U}_{\mathbf{k}'}(x, \tau; x')$$

and

$$\nabla_{\mathbf{k}} \doteq \hat{\mathbf{x}} \frac{\partial}{\partial x} + i\mathbf{k}.$$

Now we shall derive the balance equation for the flux

$$\Gamma(x, t) = \hat{\mathbf{x}} \cdot \mathbf{\Gamma}(x),$$

where

$$\mathbf{\Gamma}(x, t) \doteq \langle \delta T(\mathbf{x}, t) \delta \mathbf{u}(\mathbf{x}, t) \rangle.$$

[This function is time-dependent only because of possible initial transients; in the limit $t \rightarrow \infty$, the assumed statistical stationarity of $\mathbf{U}$ ensures that $\Gamma(x, t) = \Gamma(x)$.] From

$$\left(\frac{\partial}{\partial t} + \mathcal{L} \right) \delta T(\mathbf{x}, t) + \nabla \cdot (\delta \mathbf{u} \langle T \rangle) + \nabla \cdot (\delta \mathbf{u} \delta T - \langle \delta \mathbf{u} \delta T \rangle) = 0,$$

we solve for δT at some time t later than an arbitrary time t_0 at which we imagine imposing an initial condition:

$$\delta T(t) = G^{(0)}(t) \delta T_0 - G^{(0)}(t) \nabla \cdot [\delta \mathbf{u}(t) \langle T \rangle(t)] - G^{(0)}(t) \nabla \cdot [\delta \mathbf{u}(t) \delta T(t) - \langle \delta \mathbf{u} \delta T \rangle].$$

[We use an abbreviated notation in which $G^{(0)}(t)F(t) \equiv G^{(0)}(1, \bar{1})F(\bar{1})$.] We shall require the flux through fourth order in ϵ . Thus,

$$\mathbf{\Gamma}(t, t') = \mathbf{\Gamma}^{(2)}(t, t') + \mathbf{\Gamma}^{(4)}(t, t'),$$

where

$$\mathbf{\Gamma}^{(2)}(t, t') \doteq \langle \delta T^{(1)}(t) \delta \mathbf{u}(t') \rangle \quad (\text{C.6})$$

and

$$\mathbf{\Gamma}^{(4)}(t, t') \doteq \langle \delta T^{(3)}(t) \delta \mathbf{u}(t') \rangle. \quad (\text{C.7})$$

(The third-order flux $\langle \delta T^{(2)}(t) \delta \mathbf{u}(t') \rangle$ vanishes, since $\delta T^{(2)} = \mathcal{O}(\delta u^2)$ and odd moments of $\delta \mathbf{u}$ vanish by the Gaussian assumption. This is one of the important differences between this passive calculation and the self-consistent problems, where $\delta \mathbf{u}$ can itself pick up second- and third-order pieces.) We have

$$\begin{aligned} \delta T^{(1)}(t) &= G^{(0)}(t) \delta T(0) - G^{(0)}(t) \nabla \cdot [\delta \mathbf{u}(t) \langle T \rangle(t)], \\ \delta T^{(2)}(t) &= -G^{(0)}(t) \nabla \cdot [\delta \mathbf{u}(t) \delta T^{(1)}(t) - \langle \delta \mathbf{u}(t) \delta T^{(1)}(t) \rangle], \\ \delta T^{(3)}(t) &= -G^{(0)}(t) \nabla \cdot [\delta \mathbf{u}(t) \delta T^{(2)}(t)]. \end{aligned}$$

We shall henceforth ignore initial condition terms. (Their inclusion presents no difficulty, and just leads to the proper contributions from the initial transients.) Thus, one finds

$$[G^{(0)}]^{-1}\Gamma^{(2)}(1, 1') = -\nabla \cdot [\langle T \rangle(1) \mathbf{U}(1, 1')]$$

and

$$\begin{aligned} [G^{(0)}]^{-1}\Gamma^{(4)}(1, 1') &= -\nabla \cdot \langle \delta \mathbf{u}(1) \delta T^{(2)}(1) \delta \mathbf{u}(1') \rangle \\ &= \nabla \cdot \{ \langle \delta \mathbf{u}(1) G^{(0)}(1, \bar{1}) \nabla_{\bar{1}} \cdot \delta \mathbf{u}(\bar{1}) \rangle \langle \delta T^{(1)}(\bar{1}) \delta \mathbf{u}(1') \rangle \} \\ &\quad + \nabla \cdot \{ \langle \delta \mathbf{u}(1) G^{(0)}(1, \bar{1}) \nabla_{\bar{1}} \cdot \delta T^{(1)}(\bar{1}) \rangle \langle \delta \mathbf{u}(\bar{1}) \delta \mathbf{u}(1') \rangle \}. \end{aligned}$$

Again, we renormalize this by replacing $G^{(0)}$ by G . Also, we recognize from Eq. (C.6) the combination equal to $\Gamma^{(2)}$; this must be replaced by the unknown Γ . We then find

$$[G^{(0)}]^{-1}\Gamma^{(4)}(1, 1') \rightarrow -\hat{\Sigma}(1; \bar{1})\Gamma(\bar{1}, 1') + \nabla \cdot [G(1, \bar{1}) \nabla_{\bar{1}} \cdot \Gamma(\bar{1}, 1) \mathbf{U}(\bar{1}, 1')]. \quad (\text{C.8})$$

Finally, adding the results for $\Gamma^{(2)}$ and $\Gamma^{(4)}$, we have, displaying the vector indices explicitly, the final result:

$$([G^{(0)}]^{-1} + \hat{\Sigma})\Gamma_j(1, 1') = -\nabla_i [\langle T \rangle(1) U_{ij}(1, 1')] + \nabla_i [G(1, \bar{1}) \bar{\nabla}_k \Gamma_i(\bar{1}, 1) U_{kj}(\bar{1}, 1')]. \quad (\text{C.9})$$

In Eq. (C.8), the first term on the right-hand side is analogous to the term involving the so-called $\Sigma^{(d)}$ in Ref. 3. The last term is analogous to the term involving $\delta \hat{f}^{(d)}$. This latter term is necessary for proper symmetrization, as has been discussed in Refs. 42, 3, and 59.

These formulas simplify considerably for the one-dimensional reference model, where $\mathbf{u}(\mathbf{x}, t) \rightarrow u$, a random scalar constant. The equations in this limit are described and solved in Sec. 4.

APPENDIX D. NUMERICAL SOLUTION OF THE DIRECT-INTERACTION APPROXIMATION

The numerical solution of Eq. (4.6) can be obtained by straightforward finite-difference methods, at least for moderate R . Let the interval $[0, 1]$ be divided into n subintervals of length $\Delta = 1/n$; thus, $x \rightarrow x_i \doteq i\Delta$, so that $i = 0$ corresponds to $x = 0$ and $i = n$ corresponds to $x = 1$. We write $G(x; x') \rightarrow G(x_i; x'_j) \equiv G_i^j$. Spatial derivatives may be approximated by centered differences—e.g.,

$$\frac{\partial}{\partial x} G(x; x') \approx \frac{G_{i+1}^j - G_{i-1}^j}{2\Delta}$$

—and integrals may be evaluated approximately from the trapezoidal rule:

$$\int_0^1 dx F(x) \approx \sum_{i=0}^{n-1} \frac{1}{2} [F(x_i) + F(x_{i+1})] \Delta.$$

We use the form (4.8) for the nonlinear term. The resulting equation is

$$-R^{-1} \left(\frac{G_{i+1}^j - 2G_i^j + G_{i-1}^j}{\Delta^2} \right) + \frac{1}{4\Delta} \sum_{l=1}^{n-1} (G_{i+1}^{l+1} - G_{i-1}^{l+1} - G_{i+1}^{l-1} + G_{i-1}^{l-1}) G_l^j = \frac{1}{\Delta} \delta_i^j \quad (\text{D.1})$$

for $(i, j) = 1, \dots, n-1$, together with the boundary conditions

$$G_0^j = G_n^j = G_i^0 = G_i^n = 0.$$

Because G_i^j is symmetric, we need consider explicitly only the terms $j \leq i$. We can then consider G_i^j as a vector with $(n-1)n/2$ elements, so that Eq. (D.1) is a nonlinear system of equations which can be solved by standard iterative techniques; we used the facilities of the IMSL package, in particular the nonlinear secant solver ZSCNT.

Because of the boundary layers for large R , the number of equally spaced points required in this method scales like $n \sim R$. For a vector of length N , the work space required for the secant solver scales like N^2 . Since $N \sim n^2/2$, the number of required memory locations scales like R^4 ; because of the convolution, the cpu time scales like R^5 . For most of the runs described in this paper, we used $n = 30$, which required approximately 600K words of memory and somewhat less than two minutes of CRAY-1 cpu time per R . It is clear that the maximum R accessible to this essentially brute force approach is limited, and the only defense which can be made of it is that it is expeditious to program. If one were seriously interested in very large R , special techniques involving nonuniform grids or orthogonal polynomial expansions would have to be employed. The difficulties of more practical problems involving a time variable as well as several spatial variables are clear (although it should be noted that in the presence of a time variable the difficulties are ameliorated by the causal nature of the direct-interaction approximation; the final spatial dependences can be approached by causal integration forward from the initial conditions). On the other hand, we should also remark that the gross shape of G was discernible even for n as low as 5, even for large R . Experience shows that when n is too small for a given R , spurious oscillations develop and the resulting flux is too low, such that the DIA curve in Fig. 7 may even spuriously decrease at large R .

APPENDIX E. DISCUSSION OF THE LIMIT OF ZERO AUTOCORRELATION TIME

We have shown in Sec. 5 that for small K the mean concentration profiles are reasonably benign with constant gradients, except for small boundary layers near the wall. As $K \rightarrow 0$, the laminar profile is approached. Usually, one thinks of K as a measure of τ_{ac} , the fluctuation level being fixed. However, it is also possible to consider the limit $\tau_{ac} \rightarrow 0$, K finite. The mean profiles in this case are somewhat pathological, and we shall briefly discuss them here. Consider again the generalized reference model (2.15). For $\tau_{ac} \rightarrow 0$ (but K possibly finite), it is generally cited as an exact result for Gaussian statistics that

$$\frac{\partial}{\partial x} \langle \delta u(t) \delta T(x, t) \rangle = -K \frac{\partial^2}{\partial x^2} \langle T \rangle, \quad (\text{E.1})$$

so that, if we define an effective Reynolds number R^* by

$$[R^*]^{-1} \doteq R^{-1} + K,$$

the steady-state average of Eq. (2.15) becomes

$$-R^* \frac{\partial^2}{\partial x^2} \langle T \rangle(x) = 0. \quad (\text{E.2})$$

The conservation law which follows from Eq. (E.2),

$$\Gamma_{\text{tot}} = [R^*]^{-1}, \quad (\text{E.3})$$

is correct. However, for finite K it appears to be incompatible with the usual relationship between the total flux and the gradient at the wall, Eq. (2.12), because the solution of Eq. (E.2) subject to the usual boundary conditions (2.3) is the laminar profile, $\langle T \rangle(x) = 1 - x$, with constant derivative (-1) , incorrectly suggesting according to Eq. (2.12) that Γ_{tot} should be R^{-1} instead of Eq. (E.3).

In physical terms, the resolution is simple: Equation (E.1) states that the anomalous flux exists everywhere, *including* the boundary points $x = 0$ and $x = 1$, whereas Eq. (2.12) was derived under the boundary conditions (2.3), which force the anomalous flux to vanish at the boundaries. What actually happens in the present singular limit is that the gradient of the mean profile changes, only and precisely at the boundary points, from -1 to

$$\langle T \rangle'(0) = \langle T \rangle'(1) = -R[R^*]^{-1} = -(1 + RK). \quad (\text{E.4})$$

Thus, an infinitesimal boundary layer develops at the walls in order to carry the flux by classical processes; however, since the nonlinear interactions are completely local in the limit $\tau_{ac} \rightarrow 0$, the laminar profile remains unaltered in the interior.

The result (E.4) can be derived more formally by a variety of means. Although possibly not the shortest, we will sketch here a technique based on a Fourier integral solution of Eq. (2.15). Essentially, the method is a constructive one which rederives the properties of a solution based on general results from the theory of Green's functions.

Although we are working on a bounded interval, so that discrete Fourier transforms in space might seem indicated, we often prefer integral transforms applied to the explicitly bounded function

$$T_+(x, t) \doteq [H(x) - H(x-1)]T(x, t).$$

The equation of motion for T_+ is

$$\left(\frac{\partial}{\partial t} + u(t) \frac{\partial}{\partial x} - R^{-1} \frac{\partial^2}{\partial x^2} \right) T_+(x, t) = u(t) \delta(x) - R^{-1} [\delta'(x) + \delta(x) T'(0) - \delta(x-1) T'(1)].$$

The formal solution for the Fourier integral transform is

$$T_{+,k}(t) = \int_0^t d\bar{t} \tilde{G}_k(t; \bar{t}) \{ u(\bar{t}) - R^{-1} [ik + T'(0) - e^{-ik} T'(1)] \}, \quad (\text{E.5})$$

where the random infinitesimal response function is

$$\tilde{G}_k(t; t') \doteq H(t-t') \exp \left(-ik \int_{t'}^t d\bar{t} u(\bar{t}) - R^{-1} k^2 (t-t') \right)$$

and the random derivatives $T'(0)$ and $T'(1)$ are unknown. In the limit $\tau_{ac} \rightarrow 0$, the statistical average of Eq. (E.5) can be shown to be, after Fourier inversion and in the limit $t \rightarrow \infty$,

$$\langle T_+ \rangle(x) = -R^{-1} \int \frac{dk}{2\pi} e^{ikx} \left(\frac{ik[R^*]^{-1} - R^{-1} \langle T \rangle'(0) (1 - e^{-ik})}{k^2} \right), \quad (\text{E.6})$$

where the symmetry $\langle T \rangle'(0) = \langle T \rangle'(1)$ was used to eliminate $\langle T \rangle'(1)$. The quantity $\langle T \rangle'(0)$, which except for a multiplicative constant is just the total flux through the slab, can be determined by requiring that Eq. (E.6) be finite. This, in turn, requires that the apparent (first order) pole at $k = 0$ not, in fact, exist. Upon setting to zero the coefficient of the $\mathcal{O}(k^2)$ terms in the numerator, one is led to just the requirement (E.4). To complete the solution, one may evaluate Eq. (E.6) by residue theory, using a contour running from $-\infty$ to $+\infty$ which passes above the origin. [Although we have removed the singularity at $k = 0$, it is convenient to evaluate the terms in $\exp(ikx)$ and in $\exp(ik(x-1))$ individually; each term separately has a second-order pole.] One finds

$$\langle T_+ \rangle(x) = [H(x) - H(x-1)](1-x).$$

Since T_+ is restricted to the interval $x \in (0, 1)$, this derivation makes it clear that the derivative at the boundary, Eq. (E.4), can be different from its value (-1) in the interior.

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FIGURE CAPTIONS

- Figure 1. Model geometry for the passive advection problem, and typical profiles of mean concentration and of the classical and advective contributions to the conserved flux.
- Figure 2. The parameter space of Kubo number K vs. Reynolds number R , and scalings for the true solutions to the passive advection problem.
- Figure 3. For the reference model, representative realizations of the static scalar field $T(x)$ for both positive and negative values of Ru . Note laminar conduction for $R = 0$, and boundary layer effects for $|Ru|$ large.
- Figure 4. For the reference model, the exact mean concentration field $\langle T \rangle(x)$ for various Reynolds numbers R .
- Figure 5. For the reference model, spatial dependence of the exact advective flux $\Gamma(x)$ for various Reynolds numbers R .
- Figure 6. Exact fluxes for the reference model, as a function of Reynolds number: (a) total flux Γ_{tot} (heavy solid line); (b) spatially averaged advective flux $\bar{\Gamma}$ (solid line); (c) classical flux $\bar{\Gamma}_{\text{cl}}$ (chain-dotted line); (d) $N \doteq \bar{\Gamma}/\bar{\Gamma}_{\text{cl}}$ (dashed line). The dotted lines describe the point where $N = 1$.
- Figure 7. For the reference model, comparison of the exact solution for the mean advective flux (solid line) as a function of Reynolds number with (a) the variational bound (dashed line), and (b) the direct-interaction approximation (dotted line). The classical flux is also shown (chain-dotted line).
- Figure 8. For the reference model, comparison of spatial dependence of the advective flux $\Gamma(x)$ between the exact solution (solid line) and (a) the variational bound (dashed line), (b) the direct-interaction approximation (dotted line). The Reynolds number equals 5.
- Figure 9. Same as Fig. 8, but for $R = 20$.
- Figure 10. Comparison of the direct-interaction approximation for $G(x; x')$ to $G^{(1)}(x; x')$, for $R = 5$ and $x' = 0.33$.
- Figure 11. Same as Fig. 10, except that $R = 20$.
- Figure 12. Comparison of the direct-interaction approximation for $G(x; x')$ to the unperturbed Green's function $G^{(0)}$, for selected x' and $R = 5$.

Figure 13. Same as Fig. 12, except that $R = 20$.

Figure 14. The direct-interaction approximation for $G(x; x')$; $R = 20$.

Figure 15. The improved bound $\gamma(R, K)$ as a function of Kubo number for various Reynolds numbers.

Figure 16. Bounding profiles of mean concentration for the two-time constraint discussed in Sec. 5, for various K and $R = 50$.

Figure 17. Scaling of the bounds for test particle transport in stochastic magnetic fields.

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