

# Improved Rigorous Upper Bounds for Transport due to Passive Advection Described by Simple Models of Bounded Systems

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The work of J. A. Krommes and R. A. Smith on rigorous upper bounds for the turbulent transport of a passively advected scalar is extended in two directions: (1) For their "reference model," improved upper bounds are obtained by utilizing more sophisticated two-time constraints which include the effects of cross-correlations up to fourth order. Numerical solutions of the model stochastic differential equation are also obtained; they show that the new bounds compare quite favorably with the exact results, even at large Reynolds and Kubo numbers. (2) The theory is extended to take account of a *finite* spatial autocorrelation length  $L_c$ . As a reasonably generic example, the problem of particle transport due to statistically specified stochastic magnetic fields in a collisionless turbulent plasma is revisited. A bound is obtained which reduces for small  $L_c$  to the quasilinear limit and for large  $L_c$  to the strong turbulence limit, and which provides a reasonable and rigorous interpolation for intermediate values of  $L_c$ .

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**KEY WORDS:** Passive advection; bounds; optimum theory; stochastic magnetic fields; transport; variational principles.

## 1. INTRODUCTION

In this paper we explore the derivation of rigorous yet useful upper bounds for steady-state transport due to random passive advection.

It has long been recognized that the problem of obtaining an analytic theory of turbulence in fluids, plasmas, or similar nonlinear systems is extremely difficult. Usually, a statistical description is sought; in particular, one is often interested in the turbulent transport of various quantities such as particles or heat, which are described by certain two-point cross-

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correlation functions. However, straightforward averaging procedures applied directly to the nonlinear equations of motion encounter immediately the closure problem—namely, low-order moments are driven by higher-order ones, and a useful expression for the higher-order moments in terms of lower-order ones is not readily apparent. Sophisticated closures such as the direct-interaction approximation<sup>(1,2)</sup> provide such expressions, but the resulting equations are extremely complicated and are very difficult to solve either analytically or numerically. Furthermore, such closures misrepresent certain aspects of the physics; for example, they are largely ignorant of mechanisms of instability and coherent structures, if they exist.

An alternative approach to the problem of turbulent transport is the so-called “optimum theory.”<sup>(3,4)</sup> Although this method also uses statistical techniques, it is an approach quite different from the conventional closure-theoretical one. Instead of *approximating* the higher-order moments in terms of lower-order moments in order to close the moment hierarchy, the optimum theory employs a rigorous variational principle to address the question: What is the *maximum* attainable flux of some appropriate quantity, with given parameters and boundary conditions, subject to various constraints derived from the equations of motion. Although this question differs from the one usually addressed by conventional statistical closures, which try to predict the flux as accurately as possible, it is perfectly legitimate, since physically the knowledge of an upper bound certainly helps one to estimate the true answer, even if crudely. Furthermore, if one can exhibit one combination of constraints which yields a finite bound, it is guaranteed that adding an additional constraint will lead to a new bound which will be no worse than the old one. Thus, one can in principle envision a sequence of bounds, obtained by adding more and more constraints, which converges to the true answer. In practice, of course, only a few constraints will be tractable. The principal goal of the present work, as was true also of ref. 4, is to obtain experience with various constraints applied to simple yet nontrivial situations in order to better understand the utility of the method.

The original motivation for the optimum theory lay in Malkus' speculation<sup>(5)</sup> that the physical state achieved in experiments of steady-state thermal convection corresponds to the mathematical solution which maximizes the heat flux. Although this turned out to be true only in certain limiting cases, it motivated Howard<sup>(6)</sup> to ask a different, although mathematically rigorous, question: Instead of attempting to characterize or ascertain the true (physical) flux, he asked what the maximum possible flux would be, compatible with one or more constraints derived rigorously from the equations of motion. He showed how to formulate this question as a rigorous variational principle. Busse called the procedure the “optimum

theory” and reviewed<sup>(3)</sup> developments and applications of the method through 1978. Smith introduced the optimum theory to the plasma physics community with his discussion<sup>(7)</sup> of transport due to collisional drift waves. All those calculations were concerned with self-consistent problems, where all dependent variables are related to each other.

Krommes and Smith pointed out<sup>(4)</sup> that problems of passive advection, where the advecting velocity field is statistically specified instead of self-consistently determined, are also of interest. Not only do passive problems arise in various physical applications, an equally important motivation for studying them is that their reduced mathematical complexity enables one to exhibit and understand certain general characteristics of the optimum theory much more simply. Krommes and Smith considered in detail a pedagogical “reference model” for which an exact solution is available. They also discussed general features of the generic optimum problem of passive advection under the so-called “basic” constraint. However, they noted that passive problems involve one new qualitative feature—namely, a new dimensionless variable, the Kubo number,<sup>(8,2)</sup> must be introduced in order to describe the statistical nature of the temporal and spatial variation of the specified advecting field. Krommes and Smith emphasized that the effects of finite autocorrelation time and length described by the Kubo number were not captured by the basic constraint which had been used exclusively in the self-consistent problems, and they showed how to incorporate these effects into the formalism.

Although the detailed mathematical features of their work are described in Section 2, it is useful to give a few introductory remarks here. They considered the situation in which a scalar field  $T$  is passively advected by a random velocity field  $u$ , dependent only on time, in the presence of dissipation and in a bounded region. Thus, the model equation is of diffusion type with an advection term which is stochastically, not dynamically, nonlinear.<sup>(1)</sup> The (time-independent) boundary conditions for the scalar field were taken to be statistically sharp:  $T = 1$  at  $x = 0$  and  $T = 0$  at  $x = 1$ . Physically, this makes the walls infinite sources or sinks, which is sometimes appropriate in physical applications. The turbulence was assumed to be statistically stationary in time. They then proceeded as follows: First, they obtained the “basic” constraint by constructing a quadratic functional of  $\delta T(x, t)$  from the global balance of scalar variance (“energy”)  $\langle \delta T^2(x, t) \rangle / 2$ . This is a standard way of finding an “action” or Lagrangian. Then, they pointed out that this constraint does not involve the Kubo number, since it is constructed from moments at *one point* in space and time, so correlation lengths or times (two-point quantities) cannot enter. Hence the basic bound, although rigorous, behaves as though

the Kubo number were infinite. In order to incorporate the effects of finite correlations, they constructed a *two-time constraint* by multiplying the equation for the fluctuations  $\delta T(x, t)$  by  $\delta u(t')$  at a different time, averaging over the ensemble, and integrating over  $x$ . They showed that the solution of the resulting Euler–Lagrange equation not only reduces as expected to the result of the basic bound in the limit  $K \rightarrow \infty$  of strong turbulence, it also reproduces correctly the exact, quasilinear, result as  $K \rightarrow 0$ . In fact, for the reference model the new bound scales correctly in all regimes of Reynolds number and Kubo number.

For the reference model, the basic bound (or the two-time bound for  $K = \infty$ ) is no more than about 25% larger than the true answer in the worst case of infinite Reynolds number (very strong turbulence), and can be obtained quite simply. The direct-interaction approximation predicts a closer result<sup>(4)</sup> (lower than the exact answer) but requires substantial computational labor to obtain. Thus, an advantage of the optimum theory over conventional closures *can be* relatively simple algebra or numerical computations. The advantage is not so clear when two-time constraints are considered, although the rigor of the optimum theory is very appealing.

Of course, there is an infinite number of two-point constraints. Although the constraint of Krommes and Smith may well be the simplest, it is certainly not unique. One of our purposes in this paper is to explore the possibility of improving the upper bounds by adding more constraints. This can be done by including the effects of triplet and/or higher-order cross-correlations in the formulation. Indeed, we find that the upper bounds can be improved, although only after lengthy algebra. The most successful constraint we have found involves fourth-order correlations.

Although Krommes and Smith were able to obtain simply the exact result for the flux predicted by the reference model in the limit  $K \rightarrow \infty$  (because that limit involves no time dependence), they did not attempt to solve the model for finite  $K$ . In the present work we accomplish this solution by statistically averaging an ensemble of numerical solutions of the stochastic differential equation. This allows us to demonstrate that the improved bounds compare quite favorably with the true solution.

One flaw of the present calculations based on the reference model is that since there the advecting velocity field depends only on time—i.e., the correlation length is infinite—various analytic shortcuts can be taken and one worries that the manipulations may not generalize readily to the physically interesting case of finite correlation lengths. Thus, in the second part of this paper we generalize the work of Krommes and Smith by studying a system where the effects of the finite correlation lengths are important. In particular, we revisit the problem of particle transport in a turbulent plasma due to stochastic magnetic fields. This problem has been

treated extensively in the literature (see, for example, refs. 9–11), since field line stochasticity has been advanced<sup>(9)</sup> as a likely mechanism to partly explain the anomalous transport of electrons and heat in a turbulent, magnetically confined fusion plasma. Most of the work so far can be classified as closure-theoretical approximations to the passive situation,<sup>(11)</sup> although recently there have been several attempts to study the self-consistent problem.<sup>(12–14)</sup> Krommes and Smith did consider this problem as an application of the optimum theory; however, they only considered the basic constraint, which behaves as though the correlation time and lengths are infinite. We shall show that it is, in fact, possible to generalize their calculation to include both finite correlation time and, in particular, finite correlation lengths.

The rest of this paper is organized as follows. In Section 2 we show how to improve the two-time result of Krommes and Smith for the reference model by taking into account higher-order cross-correlations. Two ways of improvement are pursued. First, while Krommes and Smith annihilate a triplet cross-correlation by integrating the two-time constraint over  $x$ , we simply keep that term by not integrating, which leads us to introduce a space- as well as time-dependent Lagrange multiplier. The resulting bound is found to be improved slightly for finite Kubo number, but not improved in the limiting cases of either zero or infinite Kubo number. The reason is that in the case of vanishing Kubo number both two-time bounds are exact (quasilinear), while in the case of infinite Kubo number both two-time constraints reduce to the basic, one-time constraint and are thus redundant. Second, we show how to improve the bounds in the cases of infinite as well as finite Kubo number by adding to the constraints of Krommes and Smith another two-time constraint constructed from a fourth-order cross-correlation. The application to the stochastic field problem is described in Section 3. We discuss our results in Section 4. In Appendix A we describe our numerical solutions of the generalized reference model. In Appendix B we give a brief discussion of functional derivatives on bounded spatial domains. Finally, in Appendix C we give the detailed derivation of an optimum equation for (collisionless) transport due to stochastic magnetic fields.

## 2. IMPROVED UPPER BOUNDS FOR THE REFERENCE MODEL OF KROMMES AND SMITH

We begin this section by defining the problem which Krommes and Smith called the *reference model*. In this pedagogical problem, a scalar field  $T$  is passively advected by a centered, time-stationary, Gaussian velocity field  $u(t)$  whose statistics are specified explicitly in a one-dimensional,

bounded region, in the presence of (classical) dissipation. The imposed boundary conditions are statistically sharp:  $T=1$  at  $x=0$  and  $T=0$  at  $x=1$ ; these are sometimes called “rigid” because the fluctuation  $\delta T$  vanishes at the boundaries. This model serves as a tractable prototype for a wide variety of advection problems. The purpose of studying the very simple reference model is that in certain limits an exact solution is available<sup>(4)</sup> to which the results of the variational calculation can be compared; also, while in more complicated, physical situations the Euler–Lagrange equation must be solved numerically, for the reference model much of the algebra can be done analytically.

For purposes of clarity and comparison, we shall follow closely the notations of Krommes and Smith. Then the evolution equation of  $T$  is

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

where  $R$  is the Reynolds number and all the variables have been made dimensionless:  $u$  is normalized to  $\bar{u} \doteq \langle u^2 \rangle^{1/2}$ ,  $x$  is normalized to the width  $L$  of the region and thus is defined on the interval  $[0, 1]$ , and the time  $t$  is normalized to the eddy turnover time  $\tau_L \doteq L/\bar{u}$ . As Krommes and Smith discussed, there are three fundamental time scales: in addition to the eddy turnover time  $\tau_L$  ( $=1$  in dimensionless units), there is the hydrodynamic time  $\tau_h = R$  and the autocorrelation time  $\tau_{ac} = K$ . While the first two time scales are obtained by balancing the first term of Eq. (1) with the second and third terms, respectively, the autocorrelation time enters via the statistics of  $u$ . By means of dimensional analysis and random walk arguments, Krommes and Smith obtained several possible scalings for the dimensionless flux  $\gamma$ , namely classical ( $\gamma_{cl} \sim R^{-1}$ ), quasilinear ( $\gamma_q \sim K$ ), hydrodynamic ( $\gamma_h \sim R$ ), and strong turbulence ( $\gamma_s \sim 1$ ).

In the limit  $K = \infty$ , time dependence can be ignored in Eq. (1) and one obtains a second-order ordinary differential equation which can be solved analytically<sup>(4)</sup> for each realization of the Gaussian random number  $u$ . The general time-dependent case is more difficult. Although some progress can be made by employing Fourier transforms, we have failed to find an analytic representation of the solution which is simple enough to be averaged explicitly. However, it is possible to solve the stochastic differential equation (1) numerically. This work is described in Appendix A.

Now we proceed with a description of the bounding method. If we decompose  $T$  into the ensemble average  $\langle T \rangle(x)$  and the fluctuation  $\delta T(x, t)$ , then average Eq. (1) over the ensemble of  $u$ , we obtain a (local) balance relating flux and dissipation,

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

where we assumed statistical stationarity. (Since  $\langle u \rangle = 0$ , it is more suggestive and appropriate to write  $\delta u$  instead of  $u$ .) Obviously, the continuity equation (2) is the first member of a hierarchy of moment equations which relate lower-order moments to higher-order moments and exhibit the closure problem. It can be rewritten more usefully by integrating it once over  $x$ . Upon using the boundary conditions, we obtain the following simpler relation between the flux  $\Gamma(x, 0)$  and the (unknown) profile  $\langle T \rangle(x)$ :

$$\frac{d}{dx} \langle T \rangle(x) = R[\Gamma(x, 0) - \bar{\Gamma}(0) - R^{-1}] \tag{3}$$

where

$$\Gamma(x, \tau) \doteq \langle \delta u(t - \tau) \delta T(x, t) \rangle$$

and  $\bar{\Gamma}$  is the flux averaged over  $x$ :

$$\bar{\Gamma}(\tau) \doteq \int_0^1 dx \Gamma(x, \tau)$$

By subtracting Eq. (2) from Eq. (1) we find an exact equation for the fluctuations:

$$\begin{aligned} \frac{\partial}{\partial t} \delta T(x, t) + \delta u(t) \frac{d}{dx} \langle T \rangle(x) + \delta u(t) \frac{\partial}{\partial x} \delta T(x, t) \\ - \frac{\partial}{\partial x} \Gamma(x, 0) - R^{-1} \frac{\partial^2}{\partial x^2} \delta T(x, t) = 0 \end{aligned} \tag{4}$$

To obtain a variational functional, we begin by multiplying Eq. (4) by  $\delta T(x, t)$  (at the same time and space point) and ensemble averaging. We then obtain the “energy” balance equation

$$\Gamma(x, 0) \frac{d}{dx} \langle T \rangle + \frac{d}{dx} \left\langle \frac{1}{2} \delta u \delta T^2 \right\rangle - R^{-1} \left\langle \delta T \frac{\partial^2}{\partial x^2} \delta T \right\rangle = 0 \tag{5}$$

where “energy” is used generically for the scalar variance  $\langle \delta T^2/2 \rangle$ . The interpretations of the three terms in Eq. (5) as production, transfer, and dissipation, respectively, have been discussed by Krommes and Smith. Of course, Eq. (5), which relates the second-order moments to the third-order moment, is also part of a moment hierarchy. However, rather than attempting to close the hierarchy by approximating the triplet correlation, we proceed rigorously and *annihilate* it by integrating Eq. (5) over  $x$  and

using the rigid boundary conditions on  $\delta T$ . We obtain the equal-time constraint

$$\bar{\Gamma}(0) = R \overline{\Delta\Gamma^2} + R^{-1} \overline{\left\langle \left( \frac{\partial \delta T}{\partial x} \right)^2 \right\rangle} \tag{6}$$

where

$$\Delta\Gamma(x) \doteq \Gamma(x, 0) - \bar{\Gamma}(0)$$

bar means the integration over  $x$ , Eq. (3) was used to eliminate the mean gradient, and the last term was obtained after integration by parts. Krommes and Smith called Eq. (6) the “basic” constraint.

It is easy to show that knowledge of  $\bar{\Gamma}(0)$  determines the total flux of heat through the system.<sup>(4)</sup> Thus, one is led to the variational principle: *Maximize  $\bar{\Gamma}(0)$  under the constraint (6)*. This can be implemented most straightforwardly by introducing a Lagrange multiplier (for which we must solve self-consistently). Although this is not difficult for the reference model, it may be somewhat tedious in practice (especially in the generalizations to self-consistent situations). To attempt to circumvent this annoyance, Krommes and Smith followed Howard<sup>(6)</sup> and Busse<sup>(3)</sup> in formulating an alternative, minimum, principle in which, under the basic constraint, a Lagrange multiplier does not appear explicitly. (It vanishes for the basic constraint.) Thus, following Krommes and Smith, it turns out that the basic variational principle is to

$$\text{minimize } \mathcal{R} = \gamma \frac{R^2 \overline{\Delta\Gamma^2} + \overline{\langle (\partial \delta T / \partial x)^2 \rangle}}{\bar{\Gamma}(0)^2} \quad \text{subject to } \bar{\Gamma}(0) = \gamma \tag{7}$$

where  $\mathcal{R} = R$  at the stationary point. The resulting function  $\gamma(R)$  is the desired upper (basic) bound. The Euler–Lagrange equation which follows from Eq. (7) was solved in ref. 4 [see Eq. (2.40)]. This result, independent of the Kubo number, is shown in Fig. 1 as the chain-dashed curves  $\gamma_b$  for the three Reynolds numbers 5, 10, and 50. The remaining information in this figure will be discussed below.

Although the basic bound is quite rigorous, it is seriously flawed in general since it does not involve the Kubo number; due to the assumption of stationarity, the one-point constraint (6) involves no time dependence and cannot recognize two-time correlations. In other words, the basic bound behaves as though the Kubo number were infinite.

Clearly, to include the Kubo number in the expression of the upper bounds, one must consider two-time constraints, as was discussed by



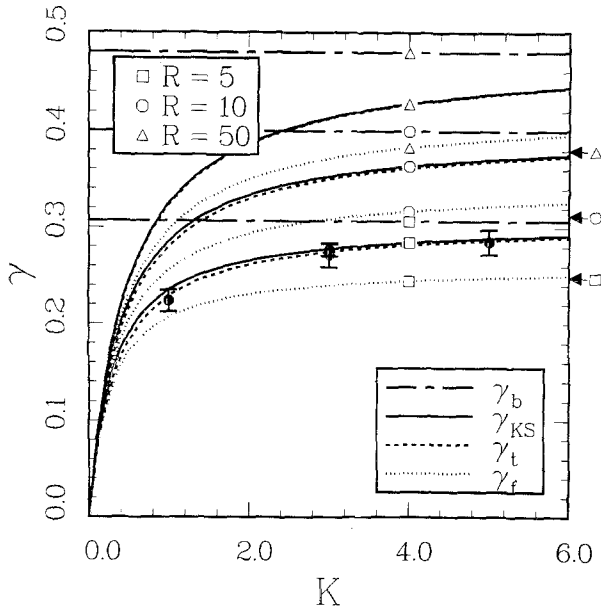


Fig. 1. Various upper bounds on  $\bar{F}$  for the reference model as a function of Kubo number  $K$ , for Reynolds numbers  $R = 5, 10$ , and  $50$ . See the text for definitions of the various curves. The solid circles with error bars are the “exact” results, from numerical integration of many realizations. The arrows indicate the exact results for  $K = \infty$ .

Krommes and Smith. They constructed a particular two-time constraint  $C_i(x, \tau)$  by multiplying Eq. (4) by  $u(t')$  and ensemble averaging to obtain

$$0 = C_i(x, \tau) \doteq \left( \frac{\partial}{\partial \tau} - R^{-1} \frac{\partial^2}{\partial x^2} \right) \Gamma(x, \tau) + U(\tau) \frac{d}{dx} \langle T \rangle + \frac{\partial}{\partial x} \mathcal{F}(x, \tau) \quad (8)$$

where  $\tau$  is the time difference variable  $\tau \doteq t - t'$ ,  $U$  is the specified auto-correlation function of  $u$ ,  $U(\tau) \doteq \langle \delta u(t) \delta u(t') \rangle = \exp(-|\tau|/K)$ ; and  $\mathcal{F}$  is a triplet cross-correlation function,  $\mathcal{F}(x, \tau) \doteq \langle \delta u(t) \delta T(x, t) \delta u(t') \rangle$ . Because this constraint is somewhat complicated, Krommes and Smith proceeded to obtain a reduced constraint  $\bar{C}_i = 0$  by integrating over  $x$  to annihilate the triplet cross-correlation. They then solved the resulting Euler–Lagrange equation and showed that the bound behaves reasonably for small Kubo number, i.e., proportional to  $K$ . (In fact, for  $K \rightarrow 0$  the bound reduces to the exact, quasilinear, result.) This bound is plotted in Fig. 1 as the solid curves  $\gamma_{KS}$ . For finite  $K$ , the new bound is smaller than the basic bound, which is expected since more constraints were applied. (However, for  $K \rightarrow \infty$  the two-time constraint asymptotes to the basic one;

thus, in that limit the new constraint is redundant and the bound is not improved.)

In fact, it is not necessary to annihilate the triplet cross-correlation in Eq. (8). A richer theory and a presumably better bound on the flux can be obtained by using the full Eq. (8) as the constraint, and this is what we shall explore here. Thus, we minimize the functional

$$\mathcal{R} = \gamma \frac{R^2 \overline{\Delta T^2} + \langle (\partial \delta T / \partial x)^2 \rangle}{\bar{F}(0)^2} + \int_{-\infty}^{\infty} d\tau \int_0^1 dx \lambda_0(x, \tau) C_t(x, \tau) + \int_0^1 dx \lambda_1(x) \langle \delta T \rangle(x) + \lambda_2 [\bar{F}(0) - \gamma] \tag{9}$$

where we take into account the constraints  $C_t = 0$ ,  $\langle \delta T \rangle = 0$ , and  $\bar{F}(0) = \gamma$  via the Lagrange multipliers  $\lambda_0$ ,  $\lambda_1$ , and  $\lambda_2$ . In the calculation of Krommes and Smith,  $\lambda_1$  and  $\lambda_2$  were omitted, as we will discuss in a moment. First, however, let us argue that the constraint  $C_t = 0$  will, in fact, lead to an improvement in the bound, rather than to just a different bound. The issue is whether the new constraint consists of the old constraint  $\bar{C}_t = 0$  plus an additional constraint—in which case the new bound cannot be worse than the old one—or whether the new constraint is simply different—in which case there is no theorem about the relation of the new bound to the old one. To show that we are, in fact, adding a further constraint to the one of Krommes and Smith, we decompose  $\lambda_0$  as

$$\lambda_0(x, \tau) = \bar{\lambda}_0(\tau) + \Delta \lambda_0(x, \tau)$$

where  $\bar{\lambda}_0$  is the spatially averaged  $\lambda_0$  and  $\Delta \lambda_0$  is the deviation from  $\bar{\lambda}_0$ . Using this, it is simple to rewrite the two-time constraint part of  $\mathcal{R}$  as

$$\int_{-\infty}^{\infty} d\tau \int_0^1 dx \lambda_0(x, \tau) C_t(x, \tau) = \int_{-\infty}^{\infty} d\tau \bar{\lambda}_0(\tau) \bar{C}_t(\tau) + \int_{-\infty}^{\infty} d\tau \int_0^1 dx \Delta \lambda_0(x, \tau) C_t(x, \tau)$$

Clearly the first term on the right-hand side is nothing but the two-time-constraint part of the functional of Krommes and Smith. Since the  $\Delta \lambda_0$  part represents another constraint additional to the old constraint of Krommes and Smith, we expect an improved bound. To ensure this, however, we must enforce the appropriate boundary conditions on  $\Delta \lambda_0$ . These can be determined by arguing that we should be able to recover the previous

bound of Krommes and Smith as we let  $\Delta\lambda_0$  vanish. Thus, in particular, we must require that  $\Delta\lambda_0$  vanishes on the boundaries:

$$\Delta\lambda_0(0, \tau) = \Delta\lambda_0(1, \tau) = 0 \tag{10}$$

In the present calculation, we must explicitly enforce the constraint  $\langle \delta T \rangle = 0$ , for the following reason. Since  $C_1$  has a cubic nonlinearity, the resulting Euler–Lagrange equation is quadratically nonlinear. Hence, in general the ensemble average of the Euler–Lagrange equation does not automatically vanish. (Krommes and Smith annihilated the cubic term, so their Euler–Lagrange equation was linear and the constraint  $\langle \delta T \rangle = 0$  was automatic; for them,  $\lambda_1 \equiv 0$ .)

The term in  $\lambda_2$  is required to ensure that the Euler–Lagrange equation satisfies the one-time constraint (6). This is *not* satisfied automatically since the two-time constraint  $C_1$  involves a constant term [when the gradient of the profile is eliminated via Eq. (3)], and this constant disappears under the functional derivative required to generate the Euler–Lagrange equation. This is a property of constraints such as  $C_1$ ; for the basic bound  $\lambda_2 = 0$  because the basic functional is homogeneous of degree 0 in  $\delta T$ . This is why Busse, Krommes and Smith, and others did not bother to introduce  $\lambda_2$  explicitly in their calculations of the basic bound. The situation is different in the two-time calculation of Krommes and Smith, where they should have included this constraint. Fortunately, their final result stands. In their calculation  $\bar{\lambda}_0$  was directly related to  $d\bar{F}/dt$ . When one includes  $\lambda_2$ , it can be shown that  $\lambda_2$  combines with  $\bar{\lambda}_0$  to give  $d\bar{F}/dt$ . Thus, the new  $\bar{\lambda}_0$  differs from that of Krommes and Smith by a constant in space; however, in terms of the new  $\bar{\lambda}_0$ , the equations for the bounding flux are the same in both calculations.

Upon taking the functional derivative of Eq. (9) with respect to  $\delta T$  and using Eq. (3), we are led to the Euler–Lagrange equation

$$\begin{aligned} 0 = & -R^{-1} \frac{\partial^2}{\partial x^2} \delta T(x, t) + \delta u(t) \frac{d}{dx} \langle T \rangle - \frac{\partial}{\partial t} \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) \delta u(t - \bar{\tau}) \\ & - R^{-1} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) \delta u(t - \bar{\tau}) + R \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) U(\bar{\tau}) \delta u(t) \\ & - R \int_{-\infty}^{\infty} d\bar{\tau} \int_0^1 d\bar{x} A_0(\bar{x}, \bar{\tau}) U(\bar{\tau}) \delta u(t) \\ & - \frac{\partial}{\partial x} \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) \delta u(t - \bar{\tau}) \delta u(t) + A_1(x) + A_2 \delta u(t) \end{aligned} \tag{11}$$

where

$$A_i \doteq \left(\frac{\gamma}{2R}\right) \lambda_i$$

This result omits various Dirac delta functions concentrated at the boundaries, because we have chosen to define  $\delta T(x, t)$  only on the open interval  $(0, 1)$ . For more discussion on this point, see Appendix B.

It is useful to proceed by eliminating the subsidiary multipliers  $A_1$  and  $A_2$  in terms of  $A_0$ . This can be done by requiring that the associated constraints be satisfied. First, by ensemble averaging Eq. (11), we can determine  $A_1$  in terms of  $A_0$ :

$$A_1(x) = \frac{\partial}{\partial x} \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) U(\bar{\tau})$$

(Note that  $A_1$  vanishes when  $A_0$  is independent of  $x$ , which is the case for the reduced constraint  $\bar{C}_t$  of Krommes and Smith.) Similarly, to find  $A_2$  in terms of  $A_0$  we multiply Eq. (11) by  $\delta T(x, t)$  (again, at equal space and time points), ensemble average, and integrate over  $x$ . Upon using the one-time constraint, we obtain

$$A_2 = -\gamma^{-1} \int_{-\infty}^{\infty} d\bar{\tau} \int_0^1 d\bar{x} A_0(\bar{x}, \bar{\tau}) U(\bar{\tau}) \tag{12}$$

(Note that  $A_2$  does not vanish even when  $A_0$  is independent of  $x$ .) Upon inserting  $A_1$  and  $A_2$  into Eq. (11), one can write the Euler-Lagrange equation much more symmetrically as

$$\begin{aligned} 0 = & -R^{-1} \frac{\partial^2}{\partial x^2} \delta T(x, t) + \delta u(t) \frac{d}{dx} \langle T \rangle - \frac{\partial}{\partial t} \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) \delta u(t - \bar{\tau}) \\ & - R^{-1} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) \delta u(t - \bar{\tau}) \\ & - \frac{\partial}{\partial x} \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) [\delta u(t - \bar{\tau}) \delta u(t) - U(\bar{\tau})] \\ & + R \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) U(\bar{\tau}) \delta u(t) \\ & - R[1 + (R\gamma)^{-1}] \int_{-\infty}^{\infty} d\bar{\tau} \int_0^1 d\bar{x} A_0(\bar{x}, \bar{\tau}) U(\bar{\tau}) \delta u(t) \tag{13} \end{aligned}$$

The remaining task is to find the undetermined Lagrange multiplier  $A_0$  self-consistently and then solve for the flux. To do this, we follow the

general procedure of Krommes and Smith, who pointed out that it is unnecessary to actually solve for  $\delta T$  itself. Rather, one can directly construct an equation for  $\Gamma$  by multiplying the Euler-Lagrange equation by  $\delta u(t')$  and ensemble averaging, using the Gaussian property of  $\delta u(t)$ . We obtain

$$0 = -R^{-1} \frac{\partial^2}{\partial x^2} \Gamma(x, \tau) + RU(\tau)[\Gamma(x, 0) - \bar{\Gamma}(0) - R^{-1}] - \left( \frac{\partial}{\partial \tau} + R^{-1} \frac{\partial^2}{\partial x^2} \right) \psi(x, \tau) + RU(\tau)[\psi(x, 0) - \bar{\psi}(0) - (R\gamma)^{-1} \bar{\psi}(0)] \quad (14)$$

where  $\psi$  is the convolution of  $A_0$  and  $U$ :

$$\psi(x, \tau) \doteq \int_{-\infty}^{\infty} d\bar{\tau} A_0(x, \bar{\tau}) U(\tau - \bar{\tau}) \quad (15)$$

Because the boundary conditions (10) imply

$$\Delta\psi(0, \tau) = \Delta\psi(1, \tau) = 0$$

where

$$\Delta\psi(x, \tau) \doteq \psi(x, \tau) - \bar{\psi}(\tau)$$

it is more convenient to express Eq. (14) in terms of  $\Delta\psi$  rather than  $\psi$  itself. To do this, we integrate Eq. (14) and  $C_t$  over  $x$  and combine the results to obtain

$$\frac{d}{d\tau} \bar{\psi}(\tau) + \gamma^{-1} \bar{\psi}(0) U(\tau) = -\frac{d}{d\tau} \bar{\Gamma}(\tau) - R^{-1} \Delta\psi'(0) U(\tau)$$

We may now use this result to eliminate  $\bar{\psi}$  in favor of  $\Delta\psi$  in Eq. (14); we finally obtain

$$0 = \frac{d}{d\tau} \bar{\Gamma}(\tau) - R^{-1} \frac{\partial^2}{\partial x^2} \Gamma(x, \tau) + RU(\tau)[\Gamma(x, 0) - \bar{\Gamma}(0) - R^{-1}] - \left( \frac{\partial}{\partial \tau} + R^{-1} \frac{\partial^2}{\partial x^2} \right) \Delta\psi(x, \tau) + RU(\tau) \Delta\psi(x, 0) - 2R^{-1} \Delta\psi'(0) U(\tau) \quad (16)$$

In obtaining the last term of Eq. (16), we used the symmetries

$$\Gamma(x, \tau) = \Gamma(1 - x, \tau), \quad \Delta\psi(x, \tau) = \Delta\psi(1 - x, \tau)$$

to deduce

$$\Delta\psi'(0) = -\Delta\psi'(1)$$

Note that for  $\Delta\psi = 0$ , Eq. (16) reduces properly to Eq. (5.17) of Krommes and Smith.

To obtain a closed set for  $\Gamma$  and  $\psi$ , we need one more equation. This may be found by multiplying Eq. (13) by  $\delta u(t) \delta u(t - \tau)$  and ensemble averaging. We obtain

$$-R^{-1} \frac{\partial^2}{\partial x^2} \mathcal{F}(x, \tau) - \frac{\partial}{\partial x} [\psi(x, \tau) + \psi(x, 0) U(\tau)] = 0 \tag{17}$$

where we used

$$\langle \delta u(t) \delta u(t - \tau) \delta u(t - \bar{\tau}) \delta u(t) \rangle - U(\tau) U(\bar{\tau}) = U(\tau - \bar{\tau}) + U(\tau) U(\bar{\tau})$$

After we integrate once over  $x$ , we can rewrite Eq. (17) in a form appropriate for use in the two-time constraint (8):

$$\frac{\partial}{\partial x} \mathcal{F}(x, \tau) = -R[\Delta\psi(x, \tau) + \Delta\psi(x, 0) U(\tau)] \tag{18}$$

Equations (8), (16), and (18) form a closed set of equations for  $\Gamma$ ,  $\Delta\psi$ , and  $\mathcal{F}$ .

If we take

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

for the autocorrelation function, we can simplify the problem by invoking separation of variables,

$$\Gamma(x, \tau) = \Gamma(x) U(\tau), \quad \Delta\psi(x, \tau) = \Delta\Psi(x) U(\tau) \tag{19}$$

In this case the Lagrange multiplier behaves in time as

$$\Delta A_0(x, \tau) = \Delta\Psi(x) \delta(\tau)$$

as can be determined by solving Eq. (15) by Fourier transforming in time. Using the expression (18) for the triplet cross-correlation together with Eqs. (19), we can reduce the constraint (8) to

$$-R^{-2} \frac{d^2}{dx^2} \Gamma + [1 + (KR)^{-1}] \Gamma - (\gamma + R^{-1}) - 2\Delta\Psi = 0 \tag{20}$$

To get the above we take  $U(\tau) = \exp(\tau/K)$ , since because of the diffusion operator the system evolves in the forward direction in time and we are

interested in the flux at  $\tau = 0$  which evolves from the state at  $\tau = -\infty$ . In the same manner we reduce Eq. (16) to

$$\begin{aligned}
 0 = & -R^{-2} \frac{d^2}{dx^2} \Gamma + \Gamma - \gamma [1 - (KR)^{-1} + (R\gamma)^{-1}] \\
 & -R^{-2} \frac{d^2}{dx^2} \Delta\Psi + [1 - (KR)^{-1}] \Delta\Psi - 2R^{-2} \Delta\Psi'(0) \quad (21)
 \end{aligned}$$

In the case when  $K \rightarrow \infty$ , one can eliminate the first two terms on the right-hand side of Eq. (21), by using Eq. (20), to arrive at an equation which involves only  $\Delta\Psi$ . One can then argue that  $\Delta\Psi = 0$ , since the equation is homogeneous in  $\Delta\Psi$  and  $\Delta\Psi = 0$  also satisfies the boundary conditions. Since the triplet cross-correlation also vanishes, we reproduce the basic result of Krommes and Smith in this case. The reason for this is that when  $K \rightarrow \infty$ , the two-time constraint reduces to the one-time constraint: The time-derivative term of Eq. (8) vanishes and the solution  $\delta T$  following the variational principle (7) satisfies Eq. (8).

The case of finite  $K$  is more involved. After straightforward algebra, one can combine Eqs. (20) and (21) to obtain

$$\begin{aligned}
 R^{-4} \frac{d^4}{dx^4} \Gamma - 4R^{-2} \frac{d^2}{dx^2} \Gamma + [3 - (KR)^{-2}] \Gamma \\
 = \{3\gamma [1 - (KR)^{-1}] + R^{-1} [3 - (KR)^{-1}]\} + 4R^{-2} \Delta\Psi'(0) \quad (22)
 \end{aligned}$$

with boundary conditions

$$\begin{aligned}
 \Gamma(x)|_{x=0,1} &= 0 \\
 R^{-2} \Gamma''(x)|_{x=0,1} &= -(\gamma + R^{-1})
 \end{aligned}$$

[The boundary conditions on  $\Gamma''$  follow by applying Eq. (10) to Eq. (20).] We can solve the above analytically: first, solve for  $\Gamma$  as a function of  $\gamma$  and  $\Delta\Psi'(0)$ ; next, use this result in Eq. (20) to obtain  $\Delta\Psi'(0)$ ; finally, integrate  $\Gamma$  over  $x$  in order to obtain an equation for  $\gamma$ . Since the final expression for  $\gamma$  is long and messy, we do not write it here. However, numerical display of the analytic solution is straightforward and is shown in Fig. 1 as the dashed curves  $\gamma_t$ . Both this and the two-time bound of Krommes and Smith behave properly for the important limiting cases:  $\gamma \sim K$  in the quasilinear regime;  $\gamma = O(1)$  in the strong turbulence regime. It is evident that our present calculations have improved the bound, although insignificantly. That  $\gamma_{KS}$  and  $\gamma_t$  should be qualitatively similar is not surprising, since the two two-time bounds are equal at the two endpoints  $K = 0$  and  $K = \infty$ .

The only way to improve the situation at  $K = \infty$  is to consider a constraint which embraces more equal-time effects, and it is natural to consider fourth-order effects. A new constraint for that purpose is obtained by multiplying Eq. (4) by  $\delta u^2(t')$  and ensemble averaging:

$$\begin{aligned}
 C_t(x, \tau) &= \left( \frac{\partial}{\partial \tau} - R^{-1} \frac{\partial^2}{\partial x^2} \right) \langle \delta u^2(t') \delta T(x, t) \rangle \\
 &\quad - \frac{d}{dx} \Gamma(x, 0) + \frac{\partial}{\partial x} \langle \delta u^2(t') \delta u(t) \delta T(x, t) \rangle \\
 &= 0
 \end{aligned}
 \tag{23}$$

The corresponding variational principle is

$$\begin{aligned}
 \text{minimize } \mathcal{R} &= \gamma \frac{R^2 \overline{\Delta T^2} + \overline{\langle (\partial \delta T / \partial x)^2 \rangle}}{\bar{\Gamma}(0)^2} + \int_{-\infty}^{\infty} d\tau \hat{\lambda}_0(\tau) \bar{C}_t(\tau) \\
 &\quad + \int_{-\infty}^{\infty} d\tau \int_0^1 dx \hat{\lambda}_1(x, \tau) C_t(x, \tau) + \int_0^1 dx \hat{\lambda}_2(x) \langle \delta T \rangle \\
 &\quad + \hat{\lambda}_3 [\bar{\Gamma}(0) - \gamma]
 \end{aligned}
 \tag{24}$$

Notice that we are using the constraint  $\bar{C}_t$ ; we are not including the triplet correlational effect in the two-time constraint equation (8), which we considered earlier. Some constraint such as  $\bar{C}_t = 0$  is required in order to ensure that the Kubo number scaling in the limit  $K \rightarrow 0$  is captured correctly. In the absence of  $\bar{C}_t$ , the resulting bound does not reduce to quasilinear theory as  $K \rightarrow 0$ .

From Eq. (24), the Euler-Lagrange equation follows as

$$\begin{aligned}
 0 &= -R^{-1} \frac{\partial^2}{\partial x^2} \delta T(x, t) + \delta u(t) \frac{d}{dx} \langle T \rangle \\
 &\quad - \int_{-\infty}^{\infty} d\bar{\tau} \bar{\Lambda}_0(\bar{\tau}) \left[ \frac{\partial}{\partial t} \delta u(t - \bar{\tau}) + \gamma^{-1} U(\bar{\tau}) \delta u(t) \right] \\
 &\quad - \left( \frac{\partial}{\partial t} + R^{-1} \frac{\partial^2}{\partial x^2} + \delta u(t) \frac{\partial}{\partial x} \right) \int_{-\infty}^{\infty} d\bar{\tau} \hat{\Lambda}_1(x, \bar{\tau}) [\delta u^2(t - \bar{\tau}) - 1]
 \end{aligned}
 \tag{25}$$

where  $\hat{\Lambda}_2$  and  $\hat{\Lambda}_3$  are determined in terms of  $\hat{\Lambda}_0$  and  $\hat{\Lambda}_1$  as before,

$$\begin{aligned}
 \hat{\Lambda}_2 &= R^{-1} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} d\bar{\tau} \hat{\Lambda}_1(x, \bar{\tau}) \\
 \hat{\Lambda}_3 &= -\gamma^{-1} \int_{-\infty}^{\infty} d\bar{\tau} \hat{\Lambda}_0(\bar{\tau}) U(\bar{\tau})
 \end{aligned}$$



The boundary conditions for  $\hat{A}_1$  are  $\hat{A}_1 = 0$  at  $x = 0$  and  $x = 1$ . Since  $\delta u$  is independent of  $\delta T$ , higher-order cross-correlations can be expressed in terms of the flux  $\Gamma$  by multiplying the Euler-Lagrange equation by the corresponding number of  $\delta u$ 's,

$$\begin{aligned}
 0 = & -R^{-1} \frac{\partial^2}{\partial x^2} \Gamma(x, \tau) + RU(\tau)[\Gamma(x, 0) - \bar{\Gamma}(0) - R^{-1}] \\
 & - \int_{-\infty}^{\infty} d\bar{\tau} \hat{A}_0(\bar{\tau}) \left[ \frac{\partial}{\partial \tau} U(\tau - \bar{\tau}) + \gamma^{-1} U(\bar{\tau}) U(\tau) \right] \\
 & - 2 \frac{\partial}{\partial x} \int_{-\infty}^{\infty} d\bar{\tau} \hat{A}_1(x, \bar{\tau}) U(\bar{\tau}) U(\tau - \bar{\tau}) \tag{26}
 \end{aligned}$$

$$\begin{aligned}
 0 = & -R^{-1} \frac{\partial^2}{\partial x^2} \langle \delta u^2(t') \delta T(x, t) \rangle \\
 & - \left( \frac{\partial}{\partial \tau} + R^{-1} \frac{\partial^2}{\partial x^2} \right) \int_{-\infty}^{\infty} d\bar{\tau} \hat{A}_1(x, \bar{\tau}) \langle \delta u^2(t') \delta u^2(t - \bar{\tau}) \rangle \tag{27}
 \end{aligned}$$

$$\begin{aligned}
 0 = & -R^{-1} \frac{\partial^2}{\partial x^2} \langle \delta u^2(t') \delta u(t'') \delta T(x, t) \rangle \\
 & + R \langle \delta u^2(t') \delta u(t'') \delta u(t) \rangle [\Gamma(x, 0) - \bar{\Gamma}(0) - R^{-1}] \\
 & - \int_{-\infty}^{\infty} d\bar{\tau} \hat{A}_0(\bar{\tau}) \left[ \frac{\partial}{\partial t} \langle \delta u^2(t') \delta u(t'') \delta u(t - \bar{\tau}) \rangle \right. \\
 & \left. + \gamma^{-1} U(\bar{\tau}) \langle \delta u^2(t') \delta u(t'') \delta u(t) \rangle \right] \\
 & - \frac{\partial}{\partial x} \int_{-\infty}^{\infty} d\bar{\tau} \hat{A}_1(x, \bar{\tau}) \\
 & \times [\langle \delta u^2(t') \delta u(t'') \delta u(t) \delta u^2(t - \bar{\tau}) \rangle - \langle \delta u^2(t') \delta u(t'') \delta u(t) \rangle] \tag{28}
 \end{aligned}$$

First of all, by integrating Eq. (26) over  $x$  and using the constraint  $\bar{C}_1 = 0$ , we find that  $\hat{A}_0$  is the same as that of Krommes and Smith. Also, assuming the temporal behavior of the Lagrange multipliers to be the Dirac delta function and separating variables, we end up with two equations, (26) and (23), where we have eliminated the triplet and fourth-order cross-correlations in favor of the flux  $\Gamma$  and the Lagrange multiplier  $\hat{A}_1$  by using Eqs. (27) and (28). An easy way to solve these coupled equations is to first solve Eq. (26) for  $\Gamma$ , then to put that expression into Eq. (23) to obtain a sixth-order, constant-coefficient ordinary differential equation for  $\Gamma$ , where the extra orders are due to the fact that we differentiate Eqs. (26) and (23)

to obtain the final differential equation. The general solution of this equation has six constants. In order to determine these constants uniquely we solve for  $\hat{A}_1$ , the triplet cross-correlation, and the fourth-order cross-correlation in terms of the constants. Then we use the boundary conditions and compare the coefficients of  $x^2$ ,  $x$ , and the constant terms of Eq. (23).

The final result is plotted in Fig. 1 as the dotted curves  $\gamma_f$ , and is seen to be significantly better than the previous ones. Also shown by the solid circles with error bars are representative points from the "exact" numerical solution of Eq. (1), described in Appendix A, for  $R = 10$ . (It is an accident that these points happen to lie close to the bound  $\gamma_{KS}$  for  $R = 5$ .) The exact results for  $K = \infty$  follow from Eq. (2.14) of Krommes and Smith and are indicated by the arrows on the right-hand ordinate. (The eye may perceive a discontinuity between the exact points at  $K = 5$  and  $K = \infty$ , but this is an illusion caused by moving the point at  $K = \infty$  into  $K = 6$ ; compare the similar situation for  $\gamma_b$  and  $\gamma_{KS}$  at  $R = 50$ .) Clearly, the newest bound leaves little room for improvement.

Although in the present case we are able to obtain the exact solution, the difficulty of that procedure actually provides a compelling argument for the bounding method. As we describe in Appendix A, it is difficult to obtain a precise value for the flux due to problems with statistical noise. Although the noise can always be reduced by using more realizations, the computations then become very long and expensive, even for the very simple, one-dimensional reference model. On the other hand, even our most complicated bound can be obtained readily and precisely by quite straightforward analytic and numerical analysis. Although it will not always be the case that the bounding method will be superior, it appears to be a viable option in a variety of problems similar to the present one.

### 3. BOUNDS ON PARTICLE TRANSPORT IN A TURBULENT PLASMA DUE TO STOCHASTIC MAGNETIC FIELDS

In the previous section, we dealt with a system where the correlation length  $L_c$  associated with the advecting velocity field was infinite. To be more realistic, we need to consider the case where the correlation length is finite. Because certain shortcuts are possible in the case of infinite  $L_c$ , it is not immediately clear how manageable the optimum theory will be in the more general situation. A specific example is the problem of particle transport due to specified stochastic magnetic fields, and we discuss that in this section. This problem was also considered by Krommes and Smith from the point of view of the optimum theory; however, they only considered the basic bound.

Since the field lines are stochastic, particles stuck to the field lines also

move in a random fashion and there results a transport of particles, energy, and so forth across the field lines.<sup>(9)</sup> However, the precise nature of this transport is subtle and depends critically on the collisionality of the particles. If the particles undergo no collisions at all, their diffusion coefficient is related straightforwardly to that of the magnetic lines, and is called the collisionless result.<sup>(15)</sup> A more interesting situation arises when the particles are allowed to diffuse along the actual lines, but are never scattered by perpendicular diffusion from their original lines. Then, the “double diffusion”<sup>(11)</sup> of the particles along the lines and of the lines themselves leads to a transport process slower than diffusive, which means that the diffusion coefficient vanishes. An even very slight amount of perpendicular diffusion, however, is sufficient<sup>(10,11)</sup> to restore a radial diffusion process for the particles, and in a wide parameter range of relevance to many experiments the “collisionless” result is again recovered. When the parallel collisionality becomes sufficiently large, other regimes and results are appropriate and Krommes *et al.*<sup>(11)</sup> have shown how these regimes are continuously connected in parameter space. Krommes and Smith considered bounds for arbitrary collisionality,<sup>(4)</sup> but since they considered only the basic bound, they were unable to obtain the collisionless scaling in the quasilinear regime of short  $L_c$ , which is of considerable experimental relevance.

To illustrate the optimum techniques for finite  $L_c$ , we shall consider a model that is most appropriate for the collisionless, quasilinear regime. Specifically, we consider the model equation<sup>(11)</sup>

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial \ell} + \delta \mathbf{u} \cdot \nabla f - R^{-1} \nabla_{\perp}^2 f = 0 \quad (29)$$

where  $\nabla_{\perp}^2 \doteq \partial^2/\partial x^2 + \partial^2/\partial y^2$ ,  $\ell$  is the arc length along the unperturbed field line,  $\partial/\partial \ell \doteq \partial/\partial z + (x/L_s) \partial/\partial y$  ( $L_s$  is the shear length),  $R \doteq \bar{u}L/\kappa_e$  is the Reynolds number, and  $\delta \mathbf{u}$  describes the stochastic field,  $\delta \mathbf{u} \doteq v \delta \mathbf{b} \equiv \hat{x} \delta u_x + \hat{y} \delta u_y$ . Here  $\delta \mathbf{b}$  is the dimensionless magnetic field fluctuation from an equilibrium configuration with good flux surfaces. We have normalized the density (defined as  $\int d\mathbf{v} f$ ) to  $n_0$  (the density at one end of the region in which we will work), the perpendicular spatial coordinates  $x$  and  $y$  to  $L$ ,  $z$  to  $L/\bar{b}$ , where  $\bar{b} \doteq \langle \delta b_x^2 \rangle^{1/2}$ , the parallel velocity  $v$  to the thermal velocity  $v_t$ , the time  $t$  to  $L/\bar{u}$ , where  $\bar{u} \doteq \bar{b}v_t$ , the particle distribution function  $f$  to the Maxwellian  $f_M$ , and the magnetic field to the average uniform field strength  $B_0$  in the  $z$  direction. In Eq. (29), the second term represents the effect of particles streaming along the unperturbed field lines and the last term describes the effects of dissipation, which we may think of<sup>(11)</sup> as modeling either real classical collisional diffusion or possibly the effect of

the  $\mathbf{E} \times \mathbf{B}$  nonlinearities in real space. Note, in particular, that we have completely omitted the effects of collisions on the parallel velocity. In the limit of infinite Reynolds number, the model correctly describes the completely collisionless (and nonphysical) situation, in which the particles never leave their original lines. In general, however, since the collision operator is absent, the model does not correspond precisely to any of the physical collisionality regimes described above, so some of the transport regimes predicted by the model are nonphysical. This is not of concern, though, since our interests here are pedagogical. The bound we shall obtain in the limit of small  $L_c$  and  $R \rightarrow \infty$  is valid for the important collisionless situation in which both the parallel and perpendicular collisionality are small, although nonzero. Thus, although the model does not completely capture the physics of a realistic experimental situation, it is rich enough to display important features and difficulties of the optimum procedure applied to passive situations with a finite autocorrelation length. There is no difficulty in principle in including the effects of parallel collisionality; see the work of Krommes and Smith.

As usual, the optimum question is: Determine bounds on the flux through a bounded region, under various rigorous constraints. Since we work in the collisionless situation, it is sufficient to determine the particle flux  $\Gamma_v$  as a function of velocity; various physical fluxes are appropriate velocity moments of  $\Gamma_v$ .

The nature of the boundary conditions we shall impose requires some discussion. Specifically, we concentrate on a region of overlapping magnetic islands, bounded by flux (KAM) surfaces which we take for simplicity of description to be planes lying at  $x = x_a$  and  $x = x_b$ . Effectively, our model calculation, in which the advecting field does not vanish at  $x = 0$  or  $x = L$ , corresponds to working in a subregion  $[0, L]$  such that  $x_a < 0 \leq x \leq L < x_b$ ; this can be thought of as an "interior slice" of a larger stochastic system. We shall impose the boundary conditions

$$n(0) = n_0, \quad n(L) = 0$$

However, for such a slice such rigid boundary conditions are inappropriate, and one is then led to question just how seriously one can take the resulting bounds. Fortunately, we can appeal to the discussion of Krommes and Smith, who argue that in the limit  $L_c \ll L$  the effects of the boundary conditions are localized near the edges of the slice and negligibly affect the global transport.

In the following, we shall exploit an important physical assumption about the perturbed magnetic field—namely, that it is perpendicular to the unperturbed  $B_z$ :

$$\delta b_z = 0$$

This approximation assumes that the field compression  $\delta(B^2)$  is negligible and, in a theory of microinstabilities, corresponds to ignoring the compressional Alfvén wave.

The structure of Eq. (29) is quite similar to that of the previous example except that here we have a three-dimensional problem and the “advecting velocity field”  $\delta\mathbf{u}$  depends on space as well as on time. Thus, the procedure we will follow is basically the same as in Section 2 except that here we will neglect the triplet and higher-order correlations: First, we find the equal-time, equal-space—i.e., one point—constraint from the “energy” balance. However, as before, this basic constraint does not describe the effects of either short autocorrelation time or length, which are important in physical situations. Thus, we add a two-point constraint to complete the variational functional. Then, we proceed in a straightforward way to obtain the Euler–Lagrange equation. The detailed calculation is described in Appendix C; the final equation for the bounding flux is

$$0 = -R^{-1} \nabla_{\perp}^2 \Gamma_v(x, x', \tilde{y}, \tilde{z}, \tau) + R[\Gamma_v(x, x, 0) - \bar{\Gamma}_v(0) - R^{-1}] \times U(x, x', \tilde{y}, \tilde{z}, \tau) + \alpha U(x, x', \tilde{y}, \tilde{z}, \tau) \tag{30}$$

where  $\Gamma_v(x, x', \tilde{y}, \tilde{z}, \tau)$  is the two-point particle flux as a function of velocity in the  $x$  direction,  $\bar{\Gamma}_v(0)$  is the one-point flux integrated over  $x$ ,  $U$  is the autocorrelation function of  $\delta u_x$ , and

$$\alpha \doteq \left[ \int_{-\infty}^{\infty} d\tilde{y} \bar{\bar{U}}(\tilde{y}, \tilde{z}, \tau) \right]^{-1} \left[ \left( \frac{\partial}{\partial \tau} + v \frac{\partial}{\partial \tilde{z}} \right) \int_{-\infty}^{\infty} d\tilde{y} \bar{\bar{F}}_v(\tilde{y}, \tilde{z}, \tau) \right]$$

Also, the double bar represents integration over both  $x$  and  $x'$ , and 0 stands for  $(\tilde{y}, \tilde{z}, \tau) = (0, 0, 0)$ . An interesting feature of this equation is that  $x'$  enters the problem as a parameter, since there is no differential operator with respect to  $x'$  in the equation; nevertheless, it is still an independent variable and the flux  $\Gamma_v$  in the second term is computed at the point  $x' = x$ . Also, notice that the coefficient  $\alpha$  of  $U$  in the last term is a constant. [See Eq. (C14).]

We can simplify the problem by choosing the correlation function to be separable and of Markovian type:

$$U(x, x', \tilde{y}, \tilde{z}, \tau) = v^2 \exp(-|x - x'|/l_x) \exp(-|\tilde{y}|/l_y) \exp(-|\tilde{z}|/l_z) \exp(-|\tau|/K)$$

where the  $l$ 's and  $K$  are the correlation lengths and correlation time, respectively. By employing separation of variables, we obtain

$$\begin{aligned}
 0 = & -R^{-2} \left( \frac{\partial^2}{\partial x^2} + l_y^{-2} \right) \Gamma_v(x, x') + v^2 [ \Gamma_v(x, x) \\
 & - \bar{\Gamma}_v(0) - R^{-1} ] \exp \left( \frac{-|x - x'|}{l_x} \right) \\
 & + R^{-1} (K^{-1} + |v| l_z^{-1}) \frac{\int_0^1 d\bar{x} d\bar{x}' \Gamma_v(\bar{x}, \bar{x}')}{\int_0^1 d\bar{x} d\bar{x}' \exp(-|\bar{x} - \bar{x}'|/l_x)} \exp \left( \frac{-|x - x'|}{l_x} \right) \quad (31)
 \end{aligned}$$

In general, we can obtain a solution  $\bar{\Gamma}_v(0)$  parametrized by  $l_x, l_y, l_z, K,$  and  $R$ .

For the extreme case that the perpendicular correlation lengths  $l_x$  and  $l_y$  are very long, Eq. (31) reduces to Eq. (5.19) of Krommes and Smith except for the factor of  $v^2$  and the streaming effect. The dimensionless bound  $\gamma$  is found to be

$$\gamma^{-1} = \gamma_\infty^{-1} + (v^2 K)^{-1} + (|v| l_z)^{-1} \quad (32)$$

where  $\gamma_\infty$  is the basic bound<sup>(4)</sup> for infinite  $K$  and  $l_z$ :

$$\gamma_\infty = R^{-1} \left[ 1 - \frac{2}{Rv} \tanh \left( \frac{Rv}{2} \right) \right] / \left[ \frac{2}{Rv} \tanh \left( \frac{Rv}{2} \right) \right]$$

For the quasilinear regime  $R \gg 1, K \ll 1,$  and  $l_z \ll 1,$  the dimensionless bound behaves as

$$\gamma \sim \min(v^2 K, |v| l_z)$$

or, after restoring the dimensions,

$$\bar{\Gamma}_v \sim \bar{b}^2 (v^2/L) \min(\tau_{ac}, l_z/|v|)$$

In the static limit, this reproduces the ‘‘Rechester–Rosenbluth’’ estimate of the diffusion coefficient  $D$  in refs. 10, 11, and 16,

$$D \sim \bar{b}^2 l_z |v|$$

and in turn the magnetic diffusion coefficient  $D_m$ :

$$D_m \sim \bar{b}^2 l_z$$

Also, it agrees with the strong turbulence scaling<sup>(4)</sup>

$$D_m \sim \bar{b} L$$

when  $R \gg 1$  and  $l_z \gg 1.$

The extreme limit where both  $l_x$  and  $l_y$  are very short is also interesting to explore. To do this, we treat the autocorrelation function as a Dirac delta function in  $x$  and  $y$ ,

$$U(x, x', \tilde{y}) = 4l_x l_y \delta(x - x') \delta(\tilde{y})$$

Rather than using Eq. (31), we go back to Eq. (30) and separate out the dependences of  $\tilde{z}$  and  $\tau$ . After some straightforward calculations it can be shown that in the strong turbulence regime the dimensionless bound  $\gamma$  scales as

$$\gamma \sim \text{const} \cdot l_x l_y Rv^2$$

and scales in the quasilinear regime as

$$\gamma^{-1} \sim \text{const} \cdot (l_x l_y v)^{-1} [(Kv)^{-1} + l_z^{-1}]$$

For finite  $l_x$ , Eq. (31) can be solved numerically. Since the solutions must resolve two disparate spatial scales,  $l_x$  and  $R^{-1}$ , straightforward computational schemes access only a limited range of  $l_x$  and  $R$ . For large Reynolds number the asymptotic solution is not readily available

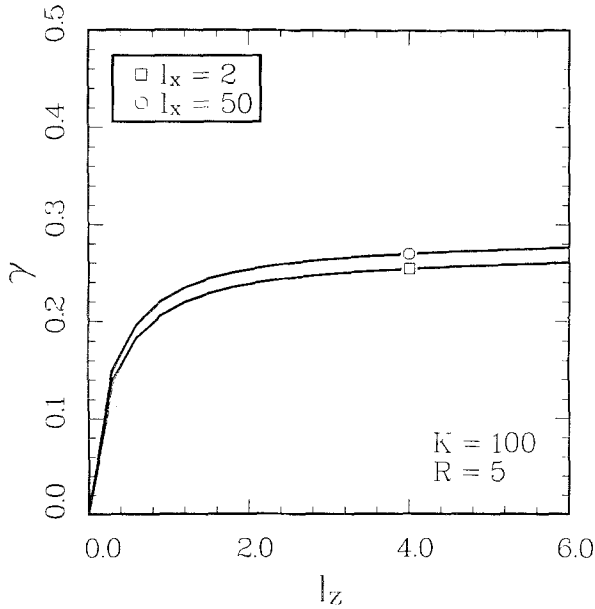


Fig. 2. Bounds for the problem of stochastic magnetic fields for two perpendicular correlation lengths  $l_x = l_y = 2$  and 50 as a function of the parallel correlation length  $l_z$  when  $K = 100$  and  $R = 5$ .

analytically; however, it is clear that a finite bound exists for infinite  $R$ . The reason is that a finite bound for infinite  $l$ 's and  $R$  can be shown to exist, and the bounds decrease with  $l_x$ ,  $l_y$ , and  $l_z$ . Figure 2 shows that the bounds are smaller for smaller perpendicular correlation length.

#### 4. CONCLUSION

In conclusion, we have considered various aspects of the theory of upper bounds for turbulent transport in passive advection problems. First, we have shown how one can generate better bounds for the reference model of Krommes and Smith by including more constraints. (This is, of course, not a new result philosophically; such improvement was already demonstrated in the original work by Howard.<sup>(6)</sup> The present work simply adds to the repertoire of examples.) When we consider the constraint which includes information up to and including the triplet cross-correlation, the improvement over the bound of Krommes and Smith is not substantial. Moreover, there is no improvement at all in the strong turbulence regime. When we add a constraint including fourth-order cross-correlations, the bounds are improved substantially in the cases of both finite and infinite Kubo number. Nevertheless, it is quite apparent that such higher-order calculations become rapidly substantially involved, even in the simple one-dimensional reference model where one has the freedom to choose appropriate statistics for the correlation of the advecting velocity field  $u$ . Thus, the utility of bounds involving the fourth-order moments for complicated practical self-consistent situations is unclear. However, in some problems where accuracy can be sacrificed in favor of crude estimates, the optimum theory with one or two constraints which recognize the effects of finite correlation time is a promising candidate for the prediction of the steady-state flux.

Second, we showed how to solve numerically the reference model for finite Kubo number. This problem is not entirely trivial, due to statistical noise. For the present problem, refined calculations of the exact solution are quite long and expensive relative to the computation of even the most complicated bound.

Finally, we applied the optimum theory to the problem of transport in a collisionless plasma due to stochastic magnetic fields. In doing this, we encountered no untoward difficulty in proceeding even when the velocity field depends on space as well as on time. We recovered already known scaling laws of the diffusion coefficient in both the quasilinear regime and the strong turbulence regime when the perpendicular correlation length is infinite. Also, we could generate numerically a family of curves of the



bounds as a function of the correlation lengths, correlation time, and the Reynolds number.

In closing, we point out that to our knowledge all of the applications thus far have been to inhomogeneous problems. Recently, Kraichnan has argued<sup>(17)</sup> that such methods can be extended to homogeneous problems as well, and to lower as well as to upper bounds. This raises the exciting possibility of rigorous bounds on the Kolmogorov constant, for example, and suggests that the bounding theory is a fruitful area for further research.

**APPENDIX A. NUMERICAL SOLUTION OF THE REFERENCE MODEL**

Here we describe direct numerical solutions of the generalized reference model (1), together with the boundary conditions

$$T(0) = 1, \quad T(1) = 0$$

The general procedure is as follows. First, we choose an arbitrary initial condition  $T(x, 0)$ , which we shall take to be the laminar profile

$$T_{\text{lam}}(x) = 1 - x$$

Next, we integrate many realizations sufficiently long that the low-order statistics such as  $\langle T \rangle$  become stationary. Finally, we compute the advective contribution  $\bar{F}$  to the flux by averaging over the realizations. As Krommes and Smith discussed,  $\bar{F}$  may be obtained from the gradient at either wall by subtracting off the classical part  $R^{-1}$ :

$$\bar{F} = -R^{-1}[\langle T \rangle'(\text{wall}) + 1]$$

The random field  $u(t)$  is assumed to be a stationary, centered, Gauss-Markov process, which is thus fully specified by its autocorrelation function

$$U(\tau) \doteq \langle \delta u(\tau) \delta u(0) \rangle = \exp(-|\tau|/K) \tag{A1}$$

Here  $K$  is the Kubo number and plays the role of the autocorrelation time  $\tau_{\text{ac}}$ . To obtain realizations of  $u(t)$ , we generate numerically an Ornstein-Uhlenbeck process (see, e.g., ref. 18), which obeys

$$\frac{du}{dt} + \nu u = a(t) \tag{A2}$$

where  $\nu = \tau_{\text{ac}}^{-1} = K^{-1}$  and  $a(t)$  is Gaussian white noise. The strength  $A$  of  $a$ , as in

$$\langle \delta a(\tau) \delta a(\tau') \rangle = A \delta(\tau - \tau')$$

can be determined from the result

$$U(t, t') = \left(\frac{A}{2v}\right) (e^{-v|t-t'|} - e^{-v(t+t')}) \tag{A3a}$$

$$\rightarrow \left(\frac{A}{2v}\right) e^{-v|t-t'|} \quad (t, t' \gg \tau_{ac} = v^{-1}) \tag{A3b}$$

by comparing Eq. (A3b) with Eq. (A1), we find  $A = 2v$ . However, we never need to generate a white noise process explicitly, since in a finite-difference scheme only the time integral of  $a$  enters. That is, from Eq. (A2)

$$u(t + \Delta t) = e^{-v \Delta t} u(t) + \Delta u(t) \tag{A4}$$

where

$$\Delta u(t) = \int_t^{t+\Delta t} dt' e^{-v(t+\Delta t-t')} a(t')$$

The increment  $\Delta u(t)$  is a centered Gaussian since  $a$  is; it is also independent of  $\Delta u$  in any other time interval. Thus, we require just the variance of  $\Delta u$ , which can be obtained from Eq. (A3a) by replacing both  $t$  and  $t'$  by  $\Delta t$ :

$$\sigma^2 \doteq \langle \Delta u(t)^2 \rangle = 1 - e^{-2v \Delta t}$$

[In the short-time limit this reduces correctly to the familiar result of velocity-space diffusion,  $\sigma^2 \rightarrow 2v \Delta t$  ( $v \Delta t \ll 1$ ).]

Thus, the final algorithm for  $u(t)$  is Eq. (A4), with

$$\Delta u(t) = \sigma \gamma(t)$$

$\gamma(t)$  being a normal random variable with zero mean and unit variance. Computer routines which generate such numbers are readily available. A typical realization of  $u(t)$  is shown in Fig. 3. The circles indicate the points computed explicitly by the previous algorithm; the solid line is generated by quasicubic Hermite interpolation (which allows a possibly discontinuous second derivative) with three segments between each circle. The mean value of  $Z = 5000$  realizations is also shown as the dotted line. In Fig. 4 we demonstrate that the generated realizations have the proper auto-correlation function. The horizontal dotted lines show the first few  $e$ -foldings  $e^{-n}$  ( $n = 1, 2, 3, 4$ ); the exact solution  $\exp(-\tau/K)$  is the diagonal dotted line. For  $Z = 1000$  one sees that the result is good through about two  $e$ -foldings, after which statistical noise sets in; for  $Z = 5000$  (not shown) the result is good through about three  $e$ -foldings.

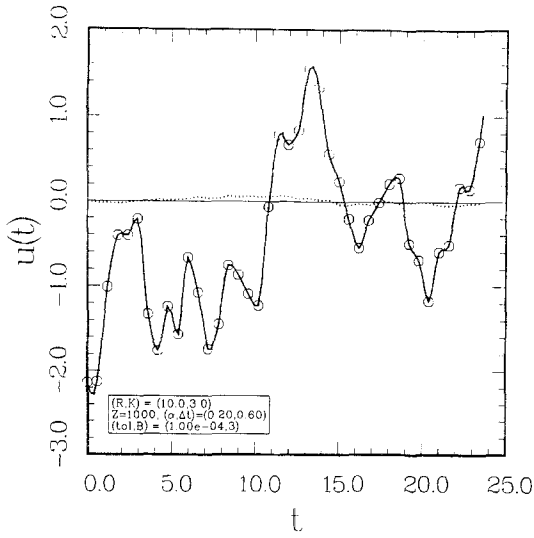


Fig. 3. A typical realization of the Ornstein-Uhlenbeck process  $u(t)$  for  $K=3$ .

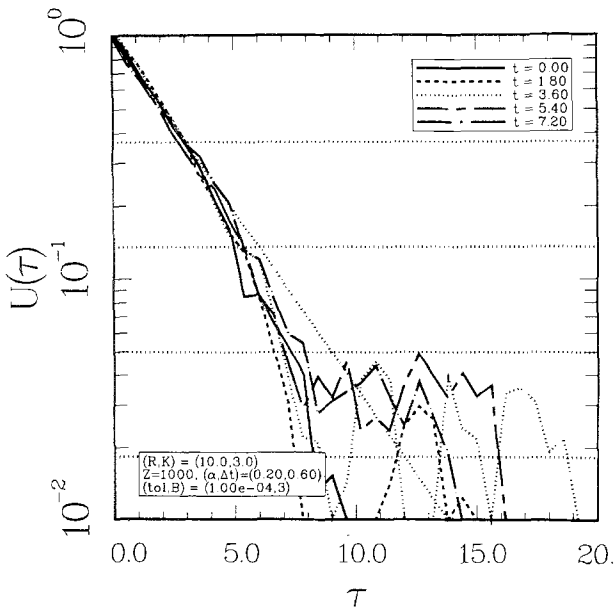


Fig. 4. Comparison of the numerically generated autocorrelation function with the expected function  $\exp(-\tau/K)$ .  $K=3$ ,  $Z=1000$ .

We relied on a commercial integration package from the International Mathematical Subroutine Library (IMSL) to integrate Eq. (1) forward in time for each realization  $u$ , in order to maintain most simply careful control of the global integration error. In space, the solutions exhibit boundary layers of width  $R^{-1}$  at the walls.<sup>(4)</sup> Thus, we employed a nonuniform mesh, with  $B$  points spaced logarithmically within each boundary layer and  $B$  more spaced uniformly between the edge of the boundary layer and the center. In other words, there were  $4B$  mesh points including the walls. Even  $B=2$  appeared to be adequate for most calculations; however, for the runs with  $Z \geq 1000$  we used  $B=3$ . Probably a small improvement in accuracy would result from a larger  $B$ . However, the integration scheme was fourth order in the average mesh spacing, and because the runs with large  $Z$  were expensive and are used only to verify that the computed bounds indeed lie above the exact solution, it was not deemed important to make more refined runs.

A typical result for the flux (averaged over all realizations) is shown in Fig. 5 as a function of time. An initial transient period is evident during which the mean profile  $\langle T \rangle$  evolves from its initial laminar form (with no advective flux) to its final steady-state value. Curves L and R represent the flux computed from the slopes at the left- and right-hand walls, respec-

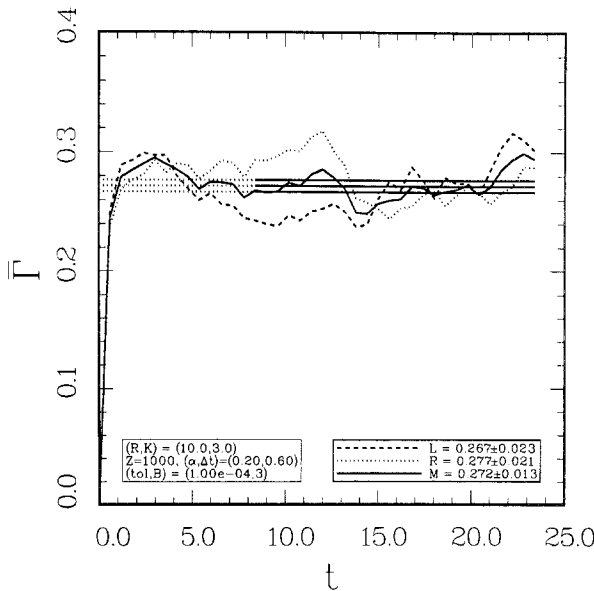


Fig. 5. Numerical solution for  $\bar{F}(t)$  at  $K=3$ , computed with  $Z=1000$  from the slope of  $\langle T \rangle$  at the left wall (L), the right wall (R), and the mean M of L and R. The time averages of the last two-thirds of the time series are shown as the solid horizontal lines.

tively. Although those values should be equal theoretically by symmetry and should be constant in the long-time limit, they differ and fluctuate in time because of statistical noise due to the finite number of realizations. Curve M is the average of curves L and R and exhibits reduced statistical fluctuations. The total integration time was determined by trial and error. It was intended to be at least three times the transient period; that, typically, was several autocorrelation times. The final values for the flux were determined from the mean of the time series of curve M during the final two-thirds of the time integration and are indicated by the solid horizontal lines. The results of several such runs are plotted for  $R = 10$  in Fig. 1 as the solid circles, with error bars determined by the sample standard deviations from the means. There are points with  $Z = 1000$  for  $K = 1$ ,  $K = 3$ , and  $K = 5$ . Each of these runs took about 1 h. of CPU time on the CRAY-2. (This time could have been reduced significantly by hand coding the time integration instead of relying on the IMSL routine; however, we opted for reliability and significantly reduced debugging time.) The point at  $K = 3$  for  $Z = 1000$ , with  $\bar{F} = 0.272 \pm 0.013$ , is almost overlaid with the result of a run for  $Z = 5000$ , which predicted  $\bar{F} = 0.277 \pm 0.006$  (and  $L \approx R \approx M$ )—in accord with the prediction of fluctuation theory that the errors scale with  $Z^{-1/2}$ . In Fig. 6 we show the mean profile at the final

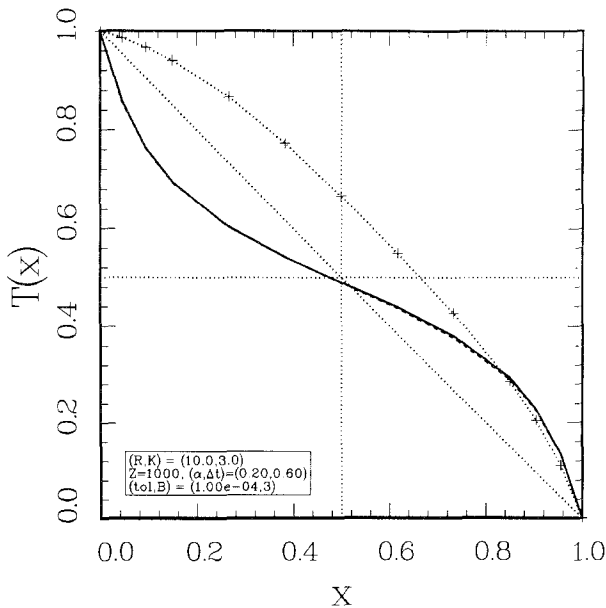


Fig. 6. For  $Z = 1000$ , the mean profile at the final time (solid line) and a typical realization (curved dotted line). The crosses indicate the spatial mesh. See text for further discussion.

integration time (solid line) and at the next-to-last time (dashed line, almost obscured by the solid line). The diagonal dotted line is the laminar profile. The curved dotted line shows a typical realization of the profile in the statistically steady state (this curve fluctuates in time around the laminar profile); the crosses indicate the mesh points. The horizontal and vertical dotted lines are intended to display any deviation of symmetry around the center. An insignificant deviation is evident for  $Z = 1000$ ; for  $Z = 5000$  (not shown), such a deviation is not visible at all.

### APPENDIX B. THE FUNCTIONAL DERIVATIVE ON BOUNDED DOMAINS

Because we work on a bounded domain in  $x$ , the final form of the Euler–Lagrange equations depends on whether one works on the open interval  $(0, 1)$  or on the closed interval  $[0, 1]$ . In particular, when one works on  $[0, 1]$ , the functional derivative gives rise to delta functions on the boundaries, which may appear difficult to deal with. Thus, we here discuss this issue in more detail.

Consider the functional

$$\mathcal{F}\{f\} \doteq \frac{1}{2} \int_0^1 d\bar{x} \left( \frac{df}{d\bar{x}} \right)^2$$

where  $f(x)$  vanishes at  $x = 0$  and  $x = 1$ . The functional derivative becomes

$$\begin{aligned} \frac{\delta \mathcal{F}}{\delta f(x)} &= - \int_0^1 d\bar{x} f''(\bar{x}) \delta(x - \bar{x}) + f'(\bar{x}) \delta(x - \bar{x}) \Big|_{\bar{x}=0}^1 \\ &= -[H(x) - H(x - 1)] f''(x) - f'(x) [\delta(x) - \delta(x - 1)] \\ &= -f''_+(x) \end{aligned}$$

where we have introduced the Heaviside function  $H(x)$  and defined the bounded function  $f_+(x)$  as

$$f_+(x) \doteq [H(x) - H(x - 1)] f(x)$$

Thus, if we work on  $(0, 1)$ , the delta functions do not appear explicitly.

As a second example, consider the functional

$$\mathcal{G}\{f\} = \int_0^1 d\bar{x} \lambda(\bar{x}) f''(\bar{x})$$

The functional derivative is

$$\begin{aligned} \frac{\delta \mathcal{G}}{\delta f(x)} &= \int_0^1 d\bar{x} \lambda''(\bar{x}) \delta(x - \bar{x}) + \lambda(\bar{x}) \delta'(x - \bar{x}) \Big|_{\bar{x}=0}^1 - \lambda'(\bar{x}) \delta(x - \bar{x}) \Big|_{\bar{x}=0}^1 \\ &= [H(x) - H(x - 1)] \lambda''(x) + 2\lambda'(x) [\delta(x) - \delta(x - 1)] \\ &\quad + \lambda(x) [\delta'(x) - \delta'(x - 1)] \\ &= \lambda''_+(x) \end{aligned}$$

The functionals  $\mathcal{F}$  and  $\mathcal{G}$  are two generic types of the functional  $\mathcal{R}$  in Section 2. Hence, it is clear that the resulting Euler–Lagrange equation in Section 2 is defined on the open interval  $(0, 1)$ .

### APPENDIX C. OPTIMUM EQUATION FOR TRANSPORT DUE TO STOCHASTIC MAGNETIC FIELDS

Here we derive a variational principle and associated Euler–Lagrange equation for the problem of collisionless particle transport due to specified stochastic magnetic fields, using a constraint which includes two-point correlations in both space and time. We begin with the model equation derived in Section 3:

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial \ell} + \delta \mathbf{u} \cdot \nabla f - R^{-1} \nabla_{\perp}^2 f = 0 \tag{C1}$$

where all symbols have been defined in the text. First, we ensemble average Eq. (C1) assuming that the turbulence is statistically stationary in time and homogeneous in the  $y$  and  $z$  directions. We obtain the continuity equation

$$\frac{d}{dx} \langle \delta u_x \delta f \rangle - R^{-1} \frac{d^2}{dx^2} \langle f \rangle = 0 \tag{C2}$$

Upon integrating once over  $x$ , we are led to

$$\frac{d}{dx} \langle f \rangle(x) = R[\Gamma_v(x, x, 0) - \bar{\Gamma}_v(0) - R^{-1}] \tag{C3}$$

where we have introduced the two fluxes

$$\Gamma_v(x, x', y - y', z - z', t - t') \doteq \langle \delta f(x, y, z, t) \delta u_x(x', y', z', t') \rangle$$

and

$$\bar{\Gamma}_v(y, z, t) \doteq \int_0^1 dx \Gamma_v(x, x, y, z, t)$$

For convenience, when no ambiguity arises, we write 0 as a shorthand for  $(y, z, t) = (0, 0, 0)$ , as in  $\bar{\Gamma}_v(0)$  in Eq. (C3). The equation for the fluctuation is

$$\left(\frac{\partial}{\partial t} + v \frac{\partial}{\partial \ell}\right) \delta f + \delta u_x \frac{d}{dx} \langle f \rangle + \nabla \cdot (\delta \mathbf{u} \delta f - \langle \delta \mathbf{u} \delta f \rangle) - R^{-1} \nabla_{\perp}^2 \delta f = 0 \quad (C4)$$

where  $\nabla \cdot \delta \mathbf{u} = 0$  was used.

We now proceed to derive the basic constraint. Upon multiplying Eq. (C4) by  $\delta f$  at the same point in space and time, we obtain

$$\Gamma_v(x, x, 0) \frac{d}{dx} \langle f \rangle + \frac{d}{dx} \langle \frac{1}{2} \delta u_x \delta f^2 \rangle - R^{-1} \langle \delta f \nabla_{\perp}^2 \delta f \rangle = 0 \quad (C5)$$

Upon using Eq. (C3) to eliminate  $d\langle f \rangle/dx$ , integrating over  $x$ , and rearranging, we are led to the basic constraint

$$\bar{\Gamma}_v(0) = R \overline{\Delta \Gamma_v^2} + R^{-1} \overline{\langle (\nabla_{\perp} \delta f)^2 \rangle} \quad (C6)$$

where

$$\Delta \Gamma_v(x) \doteq \Gamma_v(x, x, 0) - \bar{\Gamma}_v(0)$$

Thus, the basic variational principle is

$$\text{minimize } \mathcal{R} = \gamma_v \frac{R^2 \overline{\Delta \Gamma_v^2} + \overline{\langle (\nabla_{\perp} \delta f)^2 \rangle}}{\bar{\Gamma}_v(0)^2} \quad \text{subject to } \bar{\Gamma}_v(0) = \gamma_v \quad (C7)$$

To refine the bounds by including the coherence properties of the advecting stochastic field, we must use a two-point constraint. Krommes and Smith showed how to do this when the advecting field depended only on time, but here we wish to consider space dependence as well. The procedure is as follows. First, we multiply Eq. (C4) by  $\delta u_x(x', y', z', t')$  and ensemble average:

$$0 = \left(\frac{\partial}{\partial \tau} + v \frac{\partial}{\partial \ell}\right) \Gamma_v(x, x', \tilde{y}, \tilde{z}, \tau) + U(x, x', \tilde{y}, \tilde{z}, \tau) \frac{d}{dx} \langle f \rangle(x) + \nabla \cdot \mathcal{F}(x, x', \tilde{y}, \tilde{z}, \tau) - R^{-1} \nabla_{\perp}^2 \Gamma_v(x, x', \tilde{y}, \tilde{z}, \tau) \quad (C8)$$

where  $\tilde{y}$ ,  $\tilde{z}$ , and  $\tau$  are the difference variables  $\tilde{y} \doteq y - y'$ ,  $\tilde{z} \doteq z - z'$ , and  $\tau \doteq t - t'$ ,  $U$  is the autocorrelation function of  $u_x$ , and  $\mathcal{F}$  is a triplet cross-correlation function:

$$U(x, x', \tilde{y}, \tilde{z}, \tau) \doteq \langle \delta u_x(x, y, z, t) \delta u_x(x', y', z', t') \rangle$$

$$\mathcal{F}(x, x', \tilde{y}, \tilde{z}, \tau) \doteq \langle \delta \mathbf{u}(x, y, z, t) \delta f(x, y, z, t) \delta u_x(x', y', z', t') \rangle$$



After we integrate over  $x, x',$  and  $\tilde{y}$ , we immediately obtain the two-point constraint

$$0 = C(\tilde{z}, \tau) \doteq \int_{-\infty}^{\infty} d\tilde{y} \int_0^1 dx dx' \left( \frac{\partial}{\partial \tau} + v \frac{\partial}{\partial \tilde{z}} - R^{-1} \frac{\partial^2}{\partial x^2} \right) \Gamma_v(x, x', \tilde{y}, \tilde{z}, \tau) - \int_{-\infty}^{\infty} d\tilde{y} \int_0^1 dx' U(0, x', \tilde{y}, \tilde{z}, \tau) \tag{C9}$$

where we used the divergence-free property of  $\delta \mathbf{u}$  to write

$$U(x, x', \tilde{y}, \tilde{z}, \tau) \frac{d}{dx} \langle f \rangle(x) = \mathbf{V} \cdot [ \langle \delta \mathbf{u} \delta u'_x \rangle \langle f \rangle ]$$

and where the boundary conditions were used to obtain the last term of Eq. (C9). (Notice that the effect of magnetic shear is lost under the  $\tilde{y}$  integration.)

Now, we can proceed to construct the functional which is to be minimized:

$$\mathcal{R} = \gamma_v \frac{R^2 \overline{\Delta \Gamma_v^2} + \overline{\langle (\nabla_{\perp} \delta f)^2 \rangle}}{\overline{\Gamma_v(0)^2}} + \int_{-\infty}^{\infty} dt d\tilde{z} \lambda_0(\tilde{z}, \tau) C(\tilde{z}, \tau) + \lambda_1 [\overline{\Gamma_v(0)} - \gamma_v] \tag{C10}$$

In principle, the quantities in this functional should be integrated over  $v$  as well. (See the discussion by Krommes and Smith.) However, this is an issue only when collisions are taken into account. Here, since we consider the collisionless approximation, the velocity variable enters only as a parameter and we can omit the velocity integration.

The functional derivative of Eq. (46) with respect to  $\delta f$  leads to the Euler-Lagrange equation. After using Eqs. (39) and (45), we obtain

$$0 = -R^{-1} \nabla_{\perp}^2 \delta f + \delta u_x \frac{d}{dx} \langle f \rangle + A_1 \delta u_x + \int_{-\infty}^{\infty} d\bar{\tau} d\bar{z} A_0(\bar{z}, \bar{\tau}) \times \left( \frac{\partial}{\partial \bar{\tau}} + v \frac{\partial}{\partial \bar{z}} \right) \int_{-\infty}^{\infty} d\bar{y} \int_0^1 d\bar{x} \delta u_x(\bar{x}, y - \bar{y}, z - \bar{z}, t - \bar{\tau}) \tag{C11}$$

where

$$A_i = \left( \frac{\gamma_v}{2R} \right) \lambda_i$$

In the same manner as in Section 2,  $A_1$  can be related to  $A_0$  by multiplying  $\delta f$  at the same point, ensemble averaging, and integrating over  $x$ :

$$A_1 = -\gamma_v^{-1} \int_{-\infty}^{\infty} d\bar{\tau} d\bar{z} A_0(\bar{z}, \bar{\tau}) \int_{-\infty}^{\infty} d\bar{y} \int_0^1 d\bar{x} U(0, \bar{x}, \bar{y}, \bar{z}, \bar{\tau})$$

By multiplying Eq. (C11) by  $\delta u_x(x', y', z', t')$  and averaging, one can write the Euler-Lagrange equation as an equation for the flux itself:

$$0 = -R^{-1} \nabla_{\perp}^2 \Gamma_v(x, x', \tilde{y}, \tilde{z}, \tau) + U(x, x', \tilde{y}, \tilde{z}, \tau) \frac{d}{dx} \langle f \rangle - \left( \frac{\partial}{\partial \tau} + v \frac{\partial}{\partial \tilde{z}} \right) \phi(x', \tilde{z}, \tau) - \gamma_v^{-1} \phi(0) U(x, x', \tilde{y}, \tilde{z}, \tau) \quad (C12)$$

where  $\phi$  is the convolution of  $A_0$  and  $U$ :

$$\phi(x, \tilde{z}, \tau) \doteq \int_{-\infty}^{\infty} d\bar{\tau} d\bar{z} A(\bar{z}, \bar{\tau}) \int_{-\infty}^{\infty} d\bar{y} \int_0^1 d\bar{x} U(x, \bar{x}, \tilde{y} - \bar{y}, \tilde{z} - \bar{z}, \tau - \bar{\tau}) \quad (C13)$$

Notice that  $\phi$  is not a function of  $\tilde{y}$ . In order to deduce the relation between  $\phi$  and  $\Gamma_v$ , we integrate Eq. (C12) over  $x, x'$ , and  $\tilde{y}$ . Since it is assumed that the  $\tilde{y}$  integrations of  $\Gamma_v$  and  $U$  are finite, and since the integral of  $\phi$  over  $\tilde{y}$  is infinite, in order for Eq. (C12) to be satisfied we must let the third term on the right-hand side of Eq. (C12) vanish:

$$\left( \frac{\partial}{\partial t} + v \frac{\partial}{\partial \tilde{z}} \right) \phi = 0$$

This leads to

$$\phi(x, \tilde{z}, \tau) = \phi(x, \tilde{z} - v\tau)$$

After we use the constraint (C9),  $\phi(0)$  is found from the integration of Eq. (C12) to be

$$\phi(0) = -\gamma_v \left[ \int_{-\infty}^{\infty} d\bar{y} \bar{\bar{U}}(\bar{y}, \tilde{z}, \tau) \right]^{-1} \left( \frac{\partial}{\partial \tau} + v \frac{\partial}{\partial \tilde{z}} \right) \int_{-\infty}^{\infty} d\bar{y} \bar{\bar{F}}_v(\bar{y}, \tilde{z}, \tau) \quad (C14)$$

where we defined double-barred quantities as

$$\bar{\bar{f}} \doteq \int_0^1 dx dx' f(x, x')$$

The above suggests that  $\Gamma_v$  and the correlation function  $U$  have the same form as a function of  $\tilde{z}$  and  $\tau$ . Finally, after we substitute for  $\phi(0)$ , we have

$$\begin{aligned}
 0 = & -R^{-1} \nabla_{\perp}^2 \Gamma_v(x, x', \tilde{y}, \tilde{z}, \tau) + R[\Gamma_v(x, x, 0) - \bar{\Gamma}_v(0) - R^{-1}] \\
 & \times U(x, x', \tilde{y}, \tilde{z}, \tau) + \left[ \int_{-\infty}^{\infty} d\bar{y} \bar{U}(\bar{y}, \tilde{z}, \tau) \right]^{-1} \\
 & \times \left[ \left( \frac{\partial}{\partial \tau} + v \frac{\partial}{\partial \tilde{z}} \right) \int_{-\infty}^{\infty} d\bar{y} \bar{\Gamma}_v(\bar{y}, \tilde{z}, \tau) \right] U(x, x', \tilde{y}, \tilde{z}, \tau) \quad (C15)
 \end{aligned}$$

This equation is discussed further in Section 3.

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