Stieltjes integral representation of effective diffusivities in time-dependent flows

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A Stieltjes integral representation for the effective diffusivity of a passive scalar in time-dependent, incompressible flows is developed. The representation provides a summability formula for the perturbative expansion of the diffusivity in powers of the Péclet number. In particular, upper and lower bounds on the effective diffusivity are obtained from Padé approximants of the series.

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Transport enhancement is the main characteristic property of turbulent flows. It is well known that mass, momentum, and energy transport rates in turbulent velocity fields greatly exceed the corresponding molecular rates. Macroscopically, advection-diffusion of a passive scalar by an incompressible flow results in a large-scale mixing motion characterized by an effective diffusitivity. Microscopically, the dynamics of transport enhancement are related to the interplay between advection and molecular diffusion. There are few flows for which the effective diffusivity can be calculated in closed form. In particular, the weak-coupling approximation becomes exact for velocity fields having a correlation time much smaller than the typical turnover and diffusive times. Perturbative techniques are needed to treat the general case when spatial and temporal velocity correlations are both relevant, or temporal correlations are so long range that the velocity can be viewed as nearly time independent. It is a matter of importance to have rigorous expressions and estimates for effective diffusivities in incompressible flows, which apply beyond the perturbative situation of small Péclet numbers. A Stieltjes integral representation of the effective diffusivity for time-independent flows, which provides a resummation procedure valid for all Péclet numbers, was developed in [1] for this purpose. Our aim here is to show that the latter representation can be extended to the physically more interesting case of time-dependent flows. The formula obtained here is valid for all incompressible flows having homogeneous and stationary vector potentials with finite variance. As in [1], upper and lower bounds for the effective diffusivity are obtained using only a finite number of terms in the perturbative expansion of the Stieltjes integral. Another consequence of the existence of a Stieltjes integral representation is that flows that have a homogeneous and stationary vector potential with finite variance always give rise to Fickian diffusive transport at large scales.

The equation for a passive scalar advected by an incompressible velocity field is

$$\partial_t \theta + \mathbf{v} \cdot \nabla \theta = \kappa \nabla^2 \theta \ . \tag{1}$$

Here $\mathbf{v}(\mathbf{x},t)$ is a random, homogeneous, and stationary velocity field satisfying the incompressibility condition $\nabla \cdot \mathbf{v} = 0$. (Note that a deterministic periodic flow can be handled similarly.) We study the transport in a frame moving with the mean flow. In this coordinate system, the average velocity $\langle \mathbf{v} \rangle$ is zero. (Henceforth, brackets will be used to denote ensemble averaging of statistical quantities). Equation (1) depends on two nondimensional parameters: the Péclet number Pe and the ratio S between the typical sweeping time and the typical correlation time (a sort of Strouhal number), defined, respectively, as

$$\mathrm{Pe} = \frac{\langle A^2 \rangle^{1/2}}{\kappa} \quad \text{and} \quad S = \frac{l^2}{\tau \langle A^2 \rangle^{1/2}} \ . \tag{2}$$

Here, the velocity correlation length is denoted by l, the velocity correlation time is τ, and the vector potential $\mathbf{A}$ has zero average value and satisfies $\nabla \times \mathbf{A} = \mathbf{v}$ and the gauge-condition $\nabla \cdot \mathbf{A} = 0$. We shall be interested in the dynamics of (1) for time and space scales much greater than the correlation time and correlation length of the velocity field. An effective diffusion equation corresponding to (1) can be derived using multiscale techniques (homogenization) [2,3,6,7]. The effective diffusivity along an arbitrary direction $\mathbf{n}$ is then given by

$$\kappa_e = \kappa + \langle (\mathbf{v} \cdot \mathbf{n})(\mathbf{w} \cdot \mathbf{n}) \rangle \ , \tag{3}$$

where the vector field $\mathbf{w}(\mathbf{x},t)$ is the solution of the auxiliary equation

$$\partial_t \mathbf{w} + (\mathbf{v} \cdot \nabla)\mathbf{w} - \kappa \nabla^2 \mathbf{w} = -\mathbf{v} \ , \tag{4}$$

having zero average value. Equation (3) expresses the effective diffusivity as the average concentration flux across a surface normal to $\mathbf{n}$ for a scalar having an average unit gradient in the direction $\mathbf{n}$. The notations $w_n = \mathbf{w} \cdot \mathbf{n}$ and $\mathbf{E} = \nabla w_n$ are introduced for convenience. Let us now take the scalar product of (4) with $\mathbf{n}$, multiply by w_n, and average. It follows from (3) that the effective diffusivity can be expressed as

$$\kappa_e = \kappa (1 + \langle E^2 \rangle) \ . \tag{5}$$

The homogeneity and stationarity of the velocity field have been exploited to derive the latter formula. It is evident from (5) that large-scale transport is always enhanced in the presence of random incompressible velocity fields.

An equation most suitable for perturbation theory can be obtained by applying the operator $(\kappa\nabla^2)^{-1}\nabla$ to both sides of (4). The result can be written as the integral equation

$$(\mathcal{J}+i\,\mathrm{Pe}\mathcal{H})\mathbf{E}=\mathrm{Pe}\mathbf{F}\ , \qquad (6)$$

where $\mathcal{J}$ is the identity, the vector field $\mathbf{F}$ is

$$\mathbf{F}=\frac{1}{\kappa\mathrm{Pe}}\nabla^{-2}\nabla(\mathbf{v}\cdot\mathbf{n})\ , \qquad (7)$$

and the operator $\mathcal{H}$ is

$$\mathcal{H}_{jl}=\frac{i}{\kappa\mathrm{Pe}}[\nabla^{-2}\nabla_j(v_l\bullet)+\delta_{jl}\partial_t\nabla^{-2}\bullet]\ . \qquad (8)$$

Our crucial remark now is that $\mathcal{H}$ is Hermitian when operating on irrotational vector fields (like $\mathbf{E}$ and $\mathbf{F}$). The latter property was proved in [1] for the time-independent case. It is worthwhile to point out that the symmetry of the advective term in (8) follows from the incompressibility of the velocity field, i.e., the existence of a vector potential. The Hermitian property for the second term in (8) is due to the skew symmetry of the time-derivative operator.

We can give more insight into the integral equation (6) by passing to the nondimensional coordinates $\tilde{x}_i=x_i/l$, $\tilde{t}=t/\tau$, and vector potential $\mathbf{B}=\langle A^2\rangle^{-1/2}\mathbf{A}$. The force $\mathbf{F}$ and the Hermitian operator $\mathcal{H}$ can be written in the form

$$\mathbf{F}=\tilde{\nabla}^{-2}\tilde{\nabla}[(\tilde{\nabla}\times\mathbf{B})\cdot\mathbf{n}] \qquad (9)$$

and

$$\mathcal{H}_{jl}=i\{\tilde{\nabla}^{-2}\tilde{\nabla}_j[(\tilde{\nabla}\times\mathbf{B})_l\bullet]+S\delta_{jl}\tilde{\partial}_t\tilde{\nabla}^{-2}\bullet\}\ , \qquad (10)$$

where S is defined in (2) and the tilde indicates that derivatives are performed with respect to nondimensional variables. It is clear from these equations that the force and the operator appearing in (6) are independent of the Péclet number. The dependence of the problem on the parameter S occurs via (10).

To derive the Stieltjes representation for the effective diffusivity, we first consider the case when the vector potential $\mathbf{A}$ is uniformly bounded over all realizations and perform at the same time a regularization of the unbounded operator $\delta_{jl}\partial_t\nabla^{-2}\bullet$. This regularization could consist, e.g., in replacing the Fourier multiplier of this operator, $\omega/(ik^2)$, by $\omega/[i(1+\epsilon^2\omega^2)(\epsilon^2+k^2)]$ where ϵ is a small number. We can then exploit the spectral representation of the Green's function of Hermitian operators to express the solution to (6) as

$$\mathbf{E}(\mathbf{x},t)=\mathrm{Pe}\int\tilde{\sigma}(d\lambda)\boldsymbol{\psi}_\lambda(\mathbf{x},t)\frac{\langle\boldsymbol{\psi}_\lambda|\mathbf{F}\rangle}{1+i\lambda\,\mathrm{Pe}}\ . \qquad (11)$$

The vector field $\boldsymbol{\psi}_\lambda$ is an eigenfunction having the eigenvalue λ, the Dirac notation for the scalar product is used, and $\tilde{\sigma}(d\lambda)$ is the spectral density of the operator $\mathcal{H}$. From (5) and (11), it follows immediately that the field $\mathbf{E}$ satisfies

$$\langle E^2\rangle=\mathrm{Pe}^2\int\frac{\sigma(d\lambda)}{1+\mathrm{Pe}^2\lambda^2}\ , \qquad (12)$$

where $\sigma(d\lambda)$ is a probability measure since

$$\int_{-\infty}^{+\infty}\sigma(d\lambda)=\int_{-\infty}^{+\infty}\tilde{\sigma}(d\lambda)|\langle\boldsymbol{\psi}_\lambda|\mathbf{F}\rangle|^2=\langle B^2\rangle=1\ . \qquad (13)$$

Because the integral in (12) involves a probability measure, we can remove the cutoff ϵ as well as the assumption of boundedness of the vector potential and pass to the limit, as in [3]. We thus obtain the Stieltjes integral representation

$$\frac{\kappa_e}{\kappa}=1+\mathrm{Pe}^2\int\frac{\sigma(d\lambda)}{1+\mathrm{Pe}^2\lambda^2}\ . \qquad (14)$$

The moments of the measure σ are the coefficients $c_n(S)$ of the perturbation series expansion in Pe for the integral equation (6)

$$\frac{\kappa_e}{\kappa}=1+\sum_{n\geq 1}(-1)^{n-1}c_n(S)\mathrm{Pe}^{2n}\ . \qquad (15)$$

It follows from (10) that $c_n(S)$ is a polynomial of degree $2n-2$ in S. Note that the perturbation is performed around the Laplace operator, i.e., for $\mathrm{Pe}\ll 1$ and $\mathrm{Pe}/S\ll 1$. The nondimensional parameter S is thus not required to be small. As a consequence, it does not appear explicitly in (14), but it actually influences κ_e through the spectrum of the operator $\mathcal{H}$. A possible alternative would be to expand around the free diffusion operator $\partial_t-\kappa\nabla^2$, i.e., for $\mathrm{Pe}\ll 1$ with the ratio Pe/S of order 1. However, it is important to note that such an expansion does *not* lead to a Stieltjes integral representation. The reason for this is that the operator

$$i(S\tilde{\partial}_t-\tilde{\nabla}^2)^{-1}\tilde{\nabla}_j[(\tilde{\nabla}\times\mathbf{B})_l\bullet] \qquad (16)$$

is not Hermitian.

The limiting cases of the new representation, when $S\ll 1$ or $S\gg 1$, correspond, respectively, to the Stieltjes formula for time-independent velocities [1,3] and to the classical weak-coupling approximation. This is readily seen by taking the appropriate limits in (10). To obtain the limit for $S\gg 1$, note that the dominant contribution in (10) is given by the time-derivative term. The relevant limit (associated to a velocity field δ correlated in time) is $\tau\to 0$, $\bar{V}\to\infty$, with $\bar{V}^2\tau\to$const. Here, $\bar{V}$ is the rms velocity. A straightforward asymptotic analysis of (14) yields the well-known formula

$$\kappa_e=\kappa+\int_0^\infty R(\mathbf{0},t)dt\ , \qquad (17)$$

where $R(\mathbf{x},t)$ is the two-point velocity correlator.

An interesting consequence of the Stieltjes representation (14) is the fact that upper and lower bounds on the eddy diffusivity can be obtained from a finite number of terms in (15). Let us indeed denote by $\kappa_e^{(2n)}$ and $\kappa_e^{(2n-1)}$ the diagonal $[n,n]$ and the nondiagonal $[n,n-1]$ Padé approximants, respectively. The following results follow from the Stieltjes property (see, e.g., [4]): (a) The diagonal sequence increases monotonically in n; (b) The nondiagonal sequence decreases monotonically in n; (c) The Stieltjes function κ_e satisfies $\kappa_e^{(2n)}\leq\kappa_e\leq\kappa_e^{(2n-1)}$. The sequences $\kappa_e^{(2n-1)}$ and $\kappa_e^{(2n)}$ will then provide convergent upper and lower bounds on the effective diffusivity.

Moreover, the differences $\kappa_e^{(2n-1)}-\kappa_e^{(2n)}$ provide bounds on the error due to the finite order n. The latter property turns out to be useful in practical computations of effective diffusivites to estimate the convergence of the resummation procedure [5]. One important special case of the previous results is the upper bound provided by first-order perturbation theory. From (6), it follows that a sufficient condition for the existence of the effective diffusivity is

$$\langle A^2\rangle=\int\frac{\langle|\hat{v}(\mathbf{k},\omega)|^2\rangle}{k^2}d^3\mathbf{k}\,d\omega=\frac{1}{4\pi}\int\frac{R(\mathbf{x},0)}{|\mathbf{x}|}d^3\mathbf{x}<\infty\,. \tag{18}$$

Here, $\hat{v}(\mathbf{k},\omega)$ is the Fourier transform of the velocity. A homogeneous and stationary time-dependent velocity field such that its vector potential has a finite variance thus leads to a large-scale scalar transport, which is a standard diffusion process. We conclude noting that the Stieltjes integral representation for time-independent velocities derived here could be used for obtaining rigorous estimates of diffusivites in cases where both the Péclet and the Strouhal numbers defined in (2) are finite.

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