Stieltjes Integral Representation and Effective Diffusivity Bounds for Turbulent Transport

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A Stieltjes integral representation for the effective diffusivity in turbulent transport is developed. This formula is valid for all Peclet numbers and yields a rigorous resummation of the divergent perturbation series in Peclet number provided that all diagrams are computed exactly. Another consequence of the integral representation is convergent upper and lower bounds on effective diffusivity for all Peclet numbers utilizing a prescribed finite number of terms in their perturbation series.

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It is well known that the motion of a diffusive particle advected by a fluctuating velocity field is equivalent at large spatial scales and long times to an effective enhanced diffusive motion.[1] An important physical quantity in turbulent transport is the effective diffusivity coefficient at large Peclet numbers which depends on the bare particle diffusivity as well as on the velocity statistics. This quantity can be computed explicitly in very few cases and approximate procedures such as the direct interaction approximation[2] and renormalization-group methods[3-5] have been applied to compute effective diffusivity coefficients. In these approximate methods, formal diagrammatic resummation procedures are needed because the perturbation expansion in powers of Peclet number typically has a zero radius of convergence.

Here we present a new representation formula for the effective diffusivity coefficient which involves the Stieltjes integral of a probability measure and is valid for all Peclet numbers. Below we show that this formula provides a rigorous justification of the resummation of the divergent perturbation series provided that all diagrams are computed exactly. In this fashion, the representation formula provides a fundamental basis for the Kraichnan-Yakhot-Orszag resummation procedures which rely on additional approximation through a Wilson rule and/or partial resummation. We also apply the formula to develop rigorous convergent upper and lower bounds for effective diffusivity for all Peclet numbers given a finite number of coefficients in the perturbation expansion. One special case of these results is the fact that first-order perturbation theory always provides an upper bound for effective diffusivity at all Peclet numbers.

The diffusion equation for the transport of a scalar by a steady incompressible velocity field is

$$\frac{\partial T}{\partial t}+\mathbf{u}(x)\cdot\nabla T=\kappa\Delta T\,.$$

Here the velocity field $\mathbf{u}(x)$ is a stationary random field satisfying $\operatorname{div}\mathbf{u}(x)=0$ and $\langle\mathbf{u}(x)\rangle=0$ where brackets indicate ensemble averaging. The Peclet number λ, associated with this transport process, is given by

$$\lambda^2=\kappa^{-2}\int\frac{\langle|\hat{\mathbf{u}}(\mathbf{k})|^2\rangle}{|\mathbf{k}|^2}d\mathbf{k}\,, \tag{1}$$

where the caret denotes Fourier transform; we consider flows with finite λ. With the nondimensional vector potential $\boldsymbol{\Psi}$ satisfying $\operatorname{curl}\boldsymbol{\Psi}=-\mathbf{u}/\kappa\lambda$ and the matrix $\mathbf{H}$ given by $\mathbf{H}(x)\cdot=\boldsymbol{\Psi}(x)\times\cdot$, we introduce the random matrix field $\mathbf{E}$ which satisfies

$$\begin{aligned}&\nabla\cdot(\mathbf{I}+\lambda\mathbf{H})\cdot\mathbf{E}(x)=0\,,\\&\nabla\times\mathbf{E}=0\,,\\&\langle\mathbf{E}\rangle=\mathbf{I}\,.\end{aligned} \tag{2}$$

For slowly varying initial data with the form $T(x,0)=T_0(\epsilon x)$ with $\epsilon\ll 1$, the function $T(\epsilon^{-1}x,\epsilon^{-2}t)$ approaches the solution of an effective diffusive equation which describes the large time behavior. It is well known[6] that the effective diffusivity tensor is given by the renormalized diffusivity

$$\kappa_{\text{eff}}=\kappa(\mathbf{I}+\langle\tilde{\mathbf{E}}^T\cdot\tilde{\mathbf{E}}\rangle)\,, \tag{3}$$

where $\tilde{\mathbf{E}}=\mathbf{E}-\mathbf{I}$ is the fluctuating part of $\mathbf{E}$. Following Golden and Papanicolaou,[7] we utilize the matrix integral operator Γ_{ij}, $1\le i,j\le 3$, which is defined in wave-vector space as multiplication by the symbol $\hat{\Gamma}_{i,j}(k)=-k_ik_j/|\mathbf{k}|^2$ and we rewrite the first equation in (2) as the nondimensional integral equation

$$\tilde{\mathbf{E}}-\lambda\boldsymbol{\Gamma}\mathbf{H}\tilde{\mathbf{E}}=\lambda\boldsymbol{\Gamma}\mathbf{H}\mathbf{I}\,. \tag{4}$$

To derive the Stieltjes representation formula, we first consider the situation when the vector potential $\mathbf{H}(x)$ is uniformly bounded over all realizations; then the operator $\boldsymbol{\Gamma}\mathbf{H}$ defines a bounded linear operator on $L^2(\langle\cdot\rangle)$ that restricted to the subspace of zero-mean, curl-free fields, is skew symmetric. We recall that functions $f(A)$ of a skew-symmetric operator A are expressed through the resolution of the identity for A, $\{R_{i\lambda}\}$, by the spectral formula,

$$f(A)=\int_{-\infty}^{\infty} f(\lambda)\, dR_{i\lambda}.$$

By using (3) and the spectral representation of $\Gamma\mathbf{H}$ as a skew-symmetric operator, we obtain the representation formula

$$\kappa_{\text{eff}}=\kappa\left(1+\int_0^\infty \frac{\lambda^2\mu(dt)}{1+\lambda^2 t}\right). \tag{5}$$

Here $\mu(dt)$ is a positive matrix-valued measure on $[0,+\infty)$ related to the resolution of the identity dR of $\Gamma\mathbf{H}$ by

$$\mu(dt)=\langle \mathbf{H}^T\Gamma(dR_{i\sqrt{t}}+dR_{-i\sqrt{t}})\Gamma\mathbf{H}\rangle. \tag{6}$$

Below we show that $\mathrm{tr}\int\mu(dt)=1$. For periodic velocity fields the formula in (5) was suggested by Battacharya, Gupta, and Walker.[8] To obtain the representation formula for more general incompressible velocity fields with the condition that the integral in (1) is finite, we approximate by uniformly bounded fields and pass to the limit. The representation in (5) remains valid except for the fact that the representing measure may be substochastic, i.e., the measure μ satisfies $\mathrm{tr}\int\mu(dt)\le 1$. However, if the velocity potential has finite fourth moments, the equality below (6) remains valid. For statistically isotropic $u(x)$, the representation formula is

$$\kappa_{\text{eff}}/\kappa=1+\tfrac{1}{3}\int_0^\infty \frac{\lambda^2\nu(dt)}{1+\lambda^2 t}, \tag{7}$$

with $\nu(dt)=\mathrm{tr}\mu(dt)$ a probability measure. We remark that the operator $\Gamma\mathbf{H}$ is skew symmetric only because $\mathrm{div}\mathbf{v}=0$. For a slightly compressible velocity field with $\mathrm{div}\mathbf{v}\neq 0$, this operator is no longer skew symmetric and the representation formula is no longer valid.

Through (6) we compute that the moments of the representing measure $\mu(dt)$ are given in terms of the perturbation series for the integral equation in (4) by

$$\int_0^\infty t^{k-1}\mu(dt)=(-1)^{k-1}\langle \mathbf{H}(\Gamma\mathbf{H})^{2k-1}\rangle,$$

for $k=1,2,3,\ldots$; with $k=1$, we obtain $\mathrm{tr}\int\mu(dt)=1$. We restrict the remaining discussion to isotropic velocity fields. Since the measure $\nu(dt)$ in (7) is nonnegative, by expanding $(1+\lambda^2 t)^{-1}$ and integrating with respect to ν, we conclude that the partial sums, $1+\sum_{k=1}^n q_k\lambda^{2k}$, with $q_k=\frac{1}{3}\,\mathrm{tr}\langle\mathbf{H}(\Gamma\mathbf{H})^{2k-1}\rangle$ are upper bounds on $\kappa_{\text{eff}}(\lambda)/\kappa$ if n is odd and lower bounds if n is even for all Peclet numbers. The upper bound with $n=1$ yields the result that first-order perturbation theory provides an upper bound for effective diffusivity for all λ. These upper and lower bounds converge to $\kappa_{\text{eff}}(\lambda)/\kappa$ only for values of λ^2 smaller than the radius of convergence of $\sum q_k z^k$. From (7) this radius of convergence is $R=[\mathrm{lub}(\mathrm{supp}\nu)]^{-1}$. Thus, if the representing measure is not a Dirac mass at the origin, the perturbation series for effective diffusivity diverges for sufficiently large Peclet numbers; if ν has unbounded support, the radius of convergence is zero. The work of Kraichnan[2] and Yakhot and Orszag[5] suggests that for velocity fields with Gaussian statistics, the representing measure for effective diffusivity has unbounded support. Following the work of Milton[9] and Bergman[10] on effective properties of composite materials, we propose bounds for $\kappa_{\text{eff}}(\lambda^2)$ when a finite number of coefficients q_k, $k=1,2,\ldots,L$ from the perturbation series are known. These bounds are simply the $[n,n-1]$ and $[n,n]$ Padé approximants for the Stieltjes function for $\kappa_{\text{eff}}(\lambda^2)$ from (5). These rational functions of λ^2, which we denote by $\kappa^+_{2n-1}(\lambda^2)$ and $\kappa^-_{2n}(\lambda^2)$, satisfy $\kappa^-_{2n}(\lambda^2)\le\kappa_{\text{eff}}(\lambda^2)\le\kappa^+_{2n-1}(\lambda^2)$. From general principles,[11,12] these Padé approximants are known to converge for every Peclet number to $\kappa_{\text{eff}}(\lambda^2)$ as $n\to\infty$ if all moments $|q_k|$ are finite. Furthermore, $\kappa^-_{2n}(\lambda^2)$ and $\kappa^+_{2n-1}(\lambda^2)$ give the best-possible bounds for effective diffusivity based on the knowledge of q_k, $1\le k\le 2n-1$ or $2n$. There is a close formal relation between the rigorous representation formulas derived in (5) and (7) together with Padé approximations for effective diffusivity and the earlier work of Kraichnan[2] which involves a fictitious decay of probability.

The following realizability question has obvious importance. Mathematically, every probability measure $\nu(dt)$ on $[0,\infty)$ induces a potential effective diffusivity function $\kappa_{\text{eff}}(\lambda^2)$ by the formula in (7). Can every such function be realized as the effective diffusivity of advective motion by a physically reasonable incompressible velocity field? The answer is yes and the discussion is given in detail in a paper by the present authors.[13] In that paper, a variational principle for effective diffusivity is also developed along with more detailed analogies with the theory of composite materials.

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