

SPECTRAL THEORY OF ADVECTIVE DIFFUSION BY DYNAMIC AND STEADY PERIODIC FLOWS

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ABSTRACT. The analytic continuation method for representing transport in composites provides integral representations for the effective coefficients of two-phase random media. Here we adapt this method to characterize the effective thermal transport properties of advective diffusion, by steady and time-dependent, periodic flows. Our novel approach yields an integral representation for the effective diffusivity, which holds for dynamic and steady, incompressible flows, involving the spectral measure of a self-adjoint linear operator. In the case of steady fluid velocity fields, the spectral measure is associated with a Hermitian Hilbert-Schmidt integral operator, and in the case of dynamic flows, it is associated with an unbounded integro-differential operator. We utilize the integral representation to obtain asymptotic behavior of the effective diffusivity, as the molecular diffusivity tends to zero, for model, steady and dynamic flows. Our analytical results are supported by numerical computations of the spectral measures and effective diffusivities.

1. INTRODUCTION

The long time, large scale behavior of a diffusing particle or tracer being advected by an incompressible velocity field is equivalent to an enhanced diffusive process [26] with an effective diffusivity tensor κ^* . Determining the effective transport properties of advection enhanced diffusion is a challenging problem with theoretical and practical importance in many fields of science and engineering, ranging from turbulent combustion to mass, heat, and salt transport in geophysical flows [18]. A broad range of mathematical techniques have been developed that reduce the analysis of complex fluid flows, with rapidly varying structures in space and time, to solving averaged or *homogenized* equations that do not have rapidly varying data, and involve an effective parameter.

Homogenization of the advection-diffusion equation for thermal transport by time-independent, random fluid velocity fields was treated in [15]. This reduced the analysis of turbulent diffusion to solving an anisotropic diffusion equation involving a homogenized temperature and an effective diffusivity tensor κ^* . An important consequence of this analysis is that κ^* is given in terms of a *curl-free* stationary stochastic process which satisfies a steady state diffusion equation involving a skew-symmetric random matrix \mathbf{H} [2, 1]. By adapting the analytic continuation method (ACM) of homogenization theory for composites [12], it was shown that the result in [15] leads to an integral representation of κ^* , involving a spectral measure of a self-adjoint random operator [2, 1]. This integral representation of κ^* was generalized to the time-dependent case in [3, 7]. Remarkably, this method has also been extended to flows with incompressible *nonzero* effective drift [20], flows where particles diffuse according to linear collisions [21], and solute transport in porous media [6]. All these approaches yield integral representations of the symmetric and, when appropriate, the skew-symmetric part of κ^* .

Homogenization of the advection-diffusion equation for periodic or cellular, incompressible flow fields was treated in [8, 9]. As in the case of random flows, the effective diffusivity tensor κ^* is given in terms of a *curl-free* vector field which satisfies a diffusion equation involving a skew-symmetric matrix \mathbf{H} . Here, we demonstrate that the ACM can be adapted to this periodic setting to provide an integral representation for κ^* , both for steady and time-dependent flows, involving a self-adjoint linear operator and the (non-dimensional) molecular diffusivity ε . In the case of steady fluid velocity fields, the spectral measure is associated with a Hermitian Hilbert-Schmidt integral

operator involving the Green's function of the Laplacian on a square. While in the case of dynamic flows, the spectral measure is associated with a Hermitian operator which is the sum of that for steady flows and an unbounded integro-differential operator which is a composition of the time derivative and the inverse Laplacian on a square.

We utilize the analytic structure of the integral representation for κ^* to obtain its asymptotic behavior for model flows, as the molecular diffusivity ε tends to zero. This is the high Péclet number regime that is important for the understanding of transport processes in real fluid flows, where the molecular diffusivity is often quite small in comparison. In particular, FINISH THIS PARAGRAPH WHEN WE HAVE CONCRETE RESULTS. necessary and sufficient conditions for steady periodic flow fields $\kappa^* \sim \varepsilon^{1/2}$, generically, for steady flows and $\kappa^* \sim O(1)$ for “chaotic” time-dependent flows.

2. MATHEMATICAL METHODS

In this section, we formulate the effective parameter problem for enhanced diffusive transport by advective, periodic flows, and provide an integral representation for the effective diffusivity tensor κ^* , which holds for both steady and dynamic flows. The effective parameter problem [8] for such transport processes is reviewed in Section 2.1. Parallels existing between this problem of homogenization theory [4] and the ACM for representing transport in composites are put into correspondence in Section 2.2. In particular, an abstract Hilbert space framework is provided in Section 2.2.1 which places these different effective parameter problems on equal mathematical footing. Within this Hilbert space setting, we derive in Section 2.2.2 an integral representation for κ^* , involving the molecular diffusivity ε and a *spectral measure* of a self-adjoint linear operator. This integral representation is employed in Section 3 to obtain asymptotic behavior of κ^* in the scaling regime where $\varepsilon \ll 1$.

2.1. Effective transport by advective-diffusion. Consider the advection enhanced diffusive transport of a passive tracer $\phi(t, \vec{x})$, $t > 0$, $\vec{x} \in \mathbb{R}^d$, as described by the advection-diffusion equation

$$(1) \quad \partial_t \phi = \kappa_0 \Delta \phi + \vec{v} \cdot \vec{\nabla} \phi, \quad \phi(0, \vec{x}) = \phi_0(\vec{x}),$$

with $\phi_0(\vec{x})$ given. Here, ∂_t denotes partial differentiation with respect to time t , $\Delta = \vec{\nabla} \cdot \vec{\nabla} = \nabla^2$ is the Laplacian, $\kappa_0 > 0$ is the molecular diffusivity, and $\vec{v} = \vec{v}(t, \vec{x})$ is the fluid velocity field, which is assumed to be incompressible,

$$(2) \quad \vec{\nabla} \cdot \vec{v} = 0.$$

We non-dimensionalize equation (1) as follows. Let ℓ and τ be typical length and time scales associated with the problem of interest. Mapping to the non-dimensional variables $t \mapsto t/\tau$ and $x_i \mapsto x_i/\ell$, one finds that ϕ satisfies the advection-diffusion equation in (1) with a non-dimensional molecular diffusivity $\varepsilon = \tau \kappa_0 / \ell^2$ and velocity field $\vec{u} = \tau \vec{v} / \ell$, where x_i is the i^{th} component of the vector \vec{x} . Since by (2) $\vec{u}(t, \vec{x})$ is incompressible, $\vec{\nabla} \cdot \vec{u} = 0$, there is a (non-dimensional) skew-symmetric matrix $\mathbf{H}(t, \vec{x})$ such that

$$(3) \quad \vec{u} = \vec{\nabla} \cdot \mathbf{H}, \quad \mathbf{H}^T = -\mathbf{H}.$$

Using this representation of the velocity field \vec{u} , equation (1) can be written as a diffusion equation,

$$(4) \quad \partial_t \phi = \vec{\nabla} \cdot \kappa \vec{\nabla} \phi, \quad \phi(0, \vec{x}) = \phi_0(\vec{x}), \quad \kappa = \varepsilon \mathbf{I} + \mathbf{H},$$

where $\kappa(t, \vec{x}) = \varepsilon \mathbf{I} + \mathbf{H}(t, \vec{x})$ can be viewed as a local diffusivity tensor with coefficients

$$(5) \quad \kappa_{jk} = \varepsilon \delta_{jk} + H_{jk}, \quad j, k = 1, \dots, d.$$

Here, δ_{jk} is the Kronecker delta and, for notational simplicity, we denote \mathbf{I} the identity operator on all linear spaces in question.

We are interested in the dynamics of ϕ for *large* length and time scales. Anticipating that ϕ will have diffusive dynamics, we re-scale space and time by $\vec{x} \mapsto \vec{x}/\delta$ and $t \mapsto t/\delta^2$, respectively, with $\delta \ll 1$ while keeping the initial condition $\phi(0, \vec{x}) = \phi_0(\vec{x})$ independent of δ . This is equivalent to assuming that the initial data is slowly varying relative to the velocity field \vec{u} in the unscaled variables [15, 8, 9]. For periodic diffusivity coefficients in (5) which are uniformly elliptic but not necessarily symmetric, it can be shown [8] that the associated solution $\phi^\delta(t, \vec{x}) = \phi(t/\delta^2, \vec{x}/\delta)$ of (4), involving the rescaled local diffusivity tensor $\kappa(t/\delta^2, \vec{x}/\delta)$, converges to $\bar{\phi}(t, \vec{x})$, which satisfies a diffusion equation involving a (constant) effective diffusivity tensor κ^*

$$(6) \quad \partial_t \bar{\phi} = \vec{\nabla} \cdot \kappa^* \vec{\nabla} \bar{\phi}, \quad \bar{\phi}(0, \vec{x}) = \phi_0(\vec{x}).$$

The convergence is in L^2 [8],

$$(7) \quad \lim_{\delta \rightarrow 0} \left[\sup_{0 \leq t \leq t_0} \int \left| \phi^\delta(t, \vec{x}) - \bar{\phi}(t, \vec{x}) \right|^2 d\vec{x} \right] = 0,$$

for all $t_0 < \infty$, where we have used the notation $d\vec{x} = dx_1 \cdots dx_d$ for the product Lebesgue measure.

The effective diffusivity tensor κ^* is obtained by solving the cell problem [8]

$$(8) \quad \partial_t \chi_j = \vec{\nabla} \cdot \kappa (\vec{\nabla} \chi_j + \vec{e}_j), \quad \langle \vec{\nabla} \chi_j \rangle = 0,$$

for each standard basis vector \vec{e}_j , $j = 1, \dots, d$, where $\chi_j = \chi_j(t, \vec{x}; \vec{e}_j)$, $t \in \mathcal{T}$, $\vec{x} \in \mathcal{V}$, and the bounded sets $\mathcal{T} \subset \mathbb{R}$ and $\mathcal{V} \subset \mathbb{R}^d$ define the space-time period cell $((d+1)$ -torus) $\mathcal{T} \otimes \mathcal{V}$. Equation (8) also holds [8] when the velocity field is time-independent $\vec{u} = \vec{u}(\vec{x})$, however, in this case $\partial_t \chi_j = 0$. In equation (8), $\langle \cdot \rangle$ denotes spatial averaging over \mathcal{V} in the time-independent case, and when the velocity field is time-dependent $\vec{u} = \vec{u}(t, \vec{x})$, $\langle \cdot \rangle$ denotes space-time averaging over $\mathcal{T} \otimes \mathcal{V}$. The components $\kappa_{jk}^* = \kappa^* \vec{e}_j \cdot \vec{e}_k$ of the effective diffusivity tensor are given in terms of the *curl-free* vector field $\vec{\nabla} \chi_j$ [8]

$$(9) \quad \kappa_{jk}^* = \varepsilon \langle (\vec{\nabla} \chi_j + \vec{e}_j) \cdot (\vec{\nabla} \chi_k + \vec{e}_k) \rangle = \varepsilon (\delta_{jk} + \langle \vec{\nabla} \chi_j \cdot \vec{\nabla} \chi_k \rangle).$$

Equation (9) demonstrates that the effective transport of the tracer ϕ in the principle directions \vec{e}_k , $k = 1, \dots, d$, is always enhanced by the presence of an incompressible velocity field, $\kappa_{kk}^* \geq \varepsilon$. In Section 2.2, we recast equations (8) and (9) into a form which parallels the problem of characterizing effective transport in composite media [12].

2.2. The ACM for advection enhanced diffusion by periodic flows. The ACM for representing transport in composites gives a Hilbert space formulation of the effective parameter problem and provides an integral representation for the effective transport coefficients of composite media, involving a *spectral measure* of a self-adjoint linear operator which depends only on the composite geometry [12, 19, 17]. Here, we adapt this Hilbert space formulation to treat the problem of effective transport by advection enhanced diffusion. In Section 2.2.2 we extend this method to obtain an integral representation for the effective diffusivity tensor κ^* , involving a spectral measure which depends only on the fluid velocity field \vec{u} .

Toward this goal, we write the first formula in equation (8) in a more suggestive, divergence form. Under the commutability condition $\vec{\nabla} \Delta^{-1} \partial_t = \partial_t \Delta^{-1} \vec{\nabla}$ (see Section A-1), we write [8] $\partial_t \chi_k = \Delta \Delta^{-1} \partial_t \chi_k = \vec{\nabla} \cdot (\Delta^{-1} \partial_t \mathbf{I}) \vec{\nabla} \chi_k$ and define $\vec{E}_k = \vec{\nabla} \chi_k + \vec{e}_k$ and $\sigma = \kappa - \Delta^{-1} \partial_t \mathbf{I}$. Here, the inverse operation Δ^{-1} is based on convolution with the Green's function for the Laplacian Δ and $\sigma = \kappa$ in the case of steady fluid velocity fields, $\vec{u} = \vec{u}(\vec{x})$. With these definitions, equation (8) may be written as $\vec{\nabla} \cdot \sigma \vec{E}_k = 0$, $\langle \vec{E}_k \rangle = \vec{e}_k$, which is equivalent to

$$(10) \quad \vec{\nabla} \cdot \vec{J}_k = 0, \quad \vec{\nabla} \times \vec{E}_k = 0, \quad \vec{J}_k = \sigma \vec{E}_k, \quad \langle \vec{E}_k \rangle = \vec{e}_k, \quad \sigma = ((\varepsilon - \Delta^{-1} \partial_t) \mathbf{I} + \mathbf{H}).$$

The formulas in (10) are precisely the electrostatic version of Maxwell's equations for a conductive medium [12], where \vec{E}_k and \vec{J}_k are the local electric field and current density, respectively, and σ is

the local conductivity tensor of the medium. In the ACM for composites, the effective conductivity tensor σ^* is defined as

$$(11) \quad \langle \vec{J}_k \rangle = \sigma^* \langle \vec{E}_k \rangle.$$

The linear constitutive relation $\vec{J}_k = \sigma \vec{E}_k$ in (10) relates the local intensity and flux, while the linear relation in (11) relates the mean intensity and mean flux. We demonstrate in Section 2.2.1 that, for *time-independent* velocity fields \vec{u} , the definition of the effective parameter given in equation (11) reduces to (9) for diagonal components. This follows by adapting the Hilbert space formulation of the ACM for composites, to treat the effective transport properties of advective diffusion by incompressible velocity fields. This abstract Hilbert space framework is the topic of Section 2.2.1.

2.2.1. Hilbert space formulation of the effective parameter problem. In this section, we discuss an abstract Hilbert space formulation of the effective parameter problem for advection enhanced diffusive transport by incompressible velocity fields. Consider the Hilbert spaces \mathcal{H}_T and \mathcal{H}_V (over the complex field \mathbb{C}) of periodic, square integrable, vector valued functions with temporal periodicity T on the interval $\mathcal{T} = (0, T)$ and spatial periodicities V_i , $i = 1, \dots, d$, on the d -dimensional region $\mathcal{V} = (0, V_1) \times \dots \times (0, V_d)$, respectively,

$$\mathcal{H}_T = \{\vec{\xi} \in \otimes_{i=1}^d L^2(\mathcal{T}) : \vec{\xi}(0) = \vec{\xi}(T)\}, \quad \mathcal{H}_V = \{\vec{\xi} \in \otimes_{i=1}^d L^2(\mathcal{V}) : \vec{\xi}(0) = \vec{\xi}(\vec{V})\},$$

where we have defined $\vec{V} = (V_1, \dots, V_d)$ and for notational convenience we denote by 0 the null element of all linear spaces in question. By the Helmholtz theorem [14, 5], the Hilbert space \mathcal{H}_V can be decomposed into orthogonal subspaces of curl-free \mathcal{H}_\times , divergence-free \mathcal{H}_\bullet , and constant \mathcal{H}_0 vector fields, with associated orthogonal projectors $\Gamma_\times = \vec{\nabla}(\Delta^{-1})\vec{\nabla} \cdot$, $\Gamma_\bullet = -\vec{\nabla} \times (\Delta^{-1})\vec{\nabla} \times$, and Γ_0 [8, 17]

$$(12) \quad \mathcal{H}_V = \mathcal{H}_\times \oplus \mathcal{H}_\bullet \oplus \mathcal{H}_0, \quad \mathbf{I} = \Gamma_\times + \Gamma_\bullet + \Gamma_0,$$

$$\mathcal{H}_\times = \{\vec{\xi} : \vec{\nabla} \times \vec{\xi} = 0 \text{ weakly}\}, \quad \mathcal{H}_\bullet = \{\vec{\xi} : \vec{\nabla} \cdot \vec{\xi} = 0 \text{ weakly}\}, \quad \mathcal{H}_0 = \{\vec{\xi} : \vec{\xi} = \langle \vec{\xi} \rangle\}.$$

From equations (8) and (9), and the condition $0 \leq \kappa_{jk}^* < \infty$, we have that $\vec{\nabla} \chi_k$ is (weakly) curl-free, mean-zero, and $\vec{\nabla} \chi_k \in \otimes_{i=1}^d L^2(\mathcal{T} \otimes \mathcal{V})$. Hence, it is natural for our analysis of the effective parameter problem for κ^* in (9), and that of the associated integral representation discussed in Section 2.2.2, to be conducted on the Hilbert space

$$(13) \quad \mathcal{H} = \{\vec{\xi} \in \mathcal{H}_T \otimes \mathcal{H}_\times : \langle \vec{\xi} \rangle = 0\},$$

with *sesquilinear* inner-product $\langle \cdot, \cdot \rangle$ defined by $\langle \vec{\xi}, \vec{\zeta} \rangle = \langle \vec{\xi} \cdot \vec{\zeta} \rangle$. Here, we have used the simplified notation $\langle \vec{\xi} \rangle = 0 \iff \langle \xi_i \rangle = 0$ for all $i = 1, \dots, d$. We henceforth assume that $\vec{\nabla} \chi_k \in \mathcal{H}$ for time-dependent velocity fields \vec{u} , and for time-independent \vec{u} we set $\mathcal{H}_T = \emptyset$ so that $\vec{\xi} \in \mathcal{H}$ implies that $\vec{\xi} \in \mathcal{H}_\times$ with $\langle \vec{\xi} \rangle = 0$. We also assume that the flow matrix \mathbf{H} is bounded in the operator norm $\|\cdot\|$ induced by the inner-product $\langle \cdot, \cdot \rangle$ [22, 25, 24],

$$(14) \quad \|\mathbf{H}\| < \infty, \text{ on all of } \mathcal{H}.$$

Before we discuss how the Hilbert space framework presented above leads to an integral representation for κ^* , we first discuss some key differences in the theory between the cases of steady and dynamic velocity fields \vec{u} . These differences are reflected in the measure underlying this integral representation for κ^* and stem from the *unboundedness* of the operator ∂_t on the Hilbert space \mathcal{H}_T [22, 25]. For steady \vec{u} , in general, equation (11) reduces to (9) for diagonal components of the effective parameter. However, for dynamic \vec{u} , this is not true in general. The details are as follows. For dynamic \vec{u} , the operator σ in (10) can be written as $\sigma = \varepsilon \mathbf{I} + \mathbf{S}$, where $\mathbf{S} = \mathbf{H} - \Delta^{-1} \partial_t \mathbf{I}$ is

skew-symmetric $\langle \mathbf{S}\vec{\xi}, \vec{\zeta} \rangle = -\langle \vec{\xi}, \mathbf{S}\vec{\zeta} \rangle$ for all $\vec{\xi}, \vec{\zeta} \in \mathcal{H}$ such that $|\langle \partial_t \vec{\xi}, \vec{\zeta} \rangle|, |\langle \vec{\xi}, \partial_t \vec{\zeta} \rangle| < \infty$ (see Section A-1 for details). This property of the operator \mathbf{S} implies that

$$(15) \quad \langle \mathbf{S}\vec{\xi} \cdot \vec{\xi} \rangle = -\langle \mathbf{S}\vec{\xi} \cdot \vec{\xi} \rangle = 0, \quad \mathbf{S} = \mathbf{H} - \Delta^{-1} \partial_t \mathbf{I},$$

for all such $\vec{\xi} \in \mathcal{H}$. In this dynamic setting, equation (15) does not hold for every $\vec{\xi} \in \mathcal{H}$, as the unbounded operator ∂_t is defined only on a proper (dense) subset of the Hilbert space \mathcal{H}_T [22], and it may be that $|\langle \partial_t \vec{\xi}, \vec{\xi} \rangle| = \infty$. In the case of a steady velocity field we have $\mathbf{S} \equiv \mathbf{H}$ and, by equation (14) and the Cauchy Schwartz inequality, $|\langle \mathbf{S}\vec{\xi}, \vec{\xi} \rangle| \leq \|\mathbf{H}\| \|\vec{\xi}\|^2 < \infty$ for all $\vec{\xi} \in \mathcal{H}$, so equation (15) holds for all $\vec{\xi} \in \mathcal{H}$.

We now use (15) to show that, in the case of steady flows, equation (11) reduces to (9) for diagonal components of the effective parameter. In this steady case $\sigma \equiv \kappa = \varepsilon \mathbf{I} + \mathbf{H}$ which, by equation (14), is bounded in operator norm for all $\varepsilon < \infty$. Consequently, $\vec{J}_k = \sigma \vec{E}_k$ in (10) satisfies $\vec{J}_k \in \mathcal{H}_\bullet$. By the Helmholtz theorem displayed in (12) and $\vec{\nabla}_{\chi_k} \in \mathcal{H}_\times$, we have $\langle \vec{J}_k \cdot \vec{\nabla}_{\chi_k} \rangle = 0$, where $\langle \cdot \rangle$ denotes spatial averaging over \mathcal{V} in this time-independent setting. Therefore, by this and equations (11) and (15), we have [8]

$$(16) \quad \sigma_{kk}^* = \sigma^* \vec{e}_k \cdot \vec{e}_k = \langle \sigma \vec{E}_k \cdot \vec{e}_k \rangle = \langle \sigma \vec{E}_k \cdot \vec{E}_k \rangle = \langle [(\varepsilon \mathbf{I} + \mathbf{S})] \vec{E}_k \cdot \vec{E}_k \rangle = \varepsilon \langle \vec{E}_k \cdot \vec{E}_k \rangle.$$

This demonstrates that, for steady flows \vec{u} , the effective parameter problem for κ^* in (8) and (9), and that of the ACM [12] in (10) and (11) are on equal mathematical footing. It is worth mentioning that, due to the skew-symmetry of $\mathbf{S} = \mathbf{H}$ for the case of a time-independent velocity field \vec{u} , the intensity-flux relationship $\vec{J}_k = \sigma \vec{E}_k = \kappa \vec{E}_k$ in (10) is similar to that of a Hall medium [13].

Another immediate consequence of equation (15), for steady \vec{u} , is the coercivity of the bilinear functional $\Phi(\vec{\xi}, \vec{\zeta}) = \langle \sigma \vec{\xi} \cdot \vec{\zeta} \rangle$ for all $\varepsilon > 0$. By equation (14), this functional is also bounded in the case of steady \vec{u} for all $\varepsilon < \infty$. Therefore, the Lax-Milgram theorem [16] provides the existence and uniqueness of a solution $\vec{\nabla}_{\chi_k} \in \mathcal{H}$ satisfying the cell problem (8), or equivalently equation (10), in this time-independent case. The details are as follows.

The distributional form of equation (8), written as $\vec{\nabla} \cdot \sigma \vec{E}_k = 0$, is given by $\langle \sigma (\vec{\nabla}_{\chi_k} + \vec{e}_k) \cdot \vec{\nabla} \zeta \rangle = 0$, where ζ is a compactly supported, infinitely differentiable function on $\mathcal{T} \otimes \mathcal{V}$, and we stress that $\vec{\nabla} \zeta$ is *curl-free*. Motivated by this, we consider the following variational problem: find $\vec{\nabla}_{\chi_k} \in \mathcal{H}$ such that

$$(17) \quad \langle \sigma (\vec{\nabla}_{\chi_k} + \vec{e}_k) \cdot \vec{\xi} \rangle = 0, \text{ for all } \vec{\xi} \in \mathcal{H}.$$

In order to directly apply the Lax-Milgram Theorem, we rewrite equation (17) as

$$(18) \quad \Phi(\vec{\nabla}_{\chi_k}, \vec{\xi}) = \langle \sigma \vec{\nabla}_{\chi_k} \cdot \vec{\xi} \rangle = -\langle \sigma \vec{e}_k \cdot \vec{\xi} \rangle = f(\vec{\xi}).$$

By equation (15) Φ is coercive, i.e.

$$(19) \quad \Phi(\vec{\xi}, \vec{\xi}) = \langle [(\varepsilon \mathbf{I} + \mathbf{S})] \vec{\xi} \cdot \vec{\xi} \rangle = \varepsilon \|\vec{\xi}\|^2 > 0, \text{ for all } \vec{\xi} \in \mathcal{H}$$

such that $\|\vec{\xi}\| \neq 0$ and $\varepsilon > 0$, where $\|\cdot\|$ is the norm induced by the inner-product $\langle \cdot, \cdot \rangle$. Recall that $\mathbf{S} = \mathbf{H}$ in this time-independent case. This, equation (14), the triangle inequality, and the Cauchy-Schwartz inequality imply that Φ is also bounded for all $\varepsilon < \infty$

$$(20) \quad \Phi(\vec{\xi}, \vec{\zeta}) \leq (\varepsilon + \|\mathbf{H}\|) \|\vec{\xi}\| \|\vec{\zeta}\| < \infty, \text{ for all } \vec{\xi} \in \mathcal{H}.$$

For the same reasons, the linear functional $f(\vec{\xi})$ in (18) is bounded for all $\vec{\xi} \in \mathcal{H}$. Therefore, the Lax-Milgram theorem [16] provides the existence of a unique $\vec{\nabla}_{\chi_k} \in \mathcal{H}$ satisfying (8) in this time-independent case.

In the time-dependent case, equation (15) hence (19) does not hold for all $\vec{\xi} \in \mathcal{H}$. Moreover, the operator ∂_t hence σ is not bounded on \mathcal{H} [22, 24], so (20) does not hold. Consequently, the Lax-Milgram theorem cannot be directly applied, and alternate techniques [10, 11] must be used

to prove the existence and uniqueness of a solution $\vec{\nabla}\chi_k \in \mathcal{H}$ satisfying the cell problem (8). This discussion illustrates key differences in the analytic structure of the effective parameter problem for κ^* , between the cases of steady and dynamic velocity fields \vec{u} , which stem from the unboundedness of the operator ∂_t on \mathcal{H}_T , hence σ on \mathcal{H} . In Section 2.2.2, we will discuss other consequences of this boundedness/unboundedness property of the operator σ , and demonstrate that it leads to significant differences in the spectral measure underlying an integral representation of κ^* .

2.2.2. Integral representation for the effective diffusivity. In this section, we employ the Hilbert space formulation of the effective parameter problem for κ^* , discussed in Section 2.2.1, and the *spectral theorem* [22, 25, 24], to provide an integral representation for κ^* involving a *spectral measure* of a self-adjoint linear operator \mathbf{M} . This integral representation follows from the resolvent formula for $\vec{\nabla}\chi_k$ involving \mathbf{M}

$$(21) \quad \vec{\nabla}\chi_k = i(-i\varepsilon\mathbf{I} - \mathbf{M})^{-1}[\mathbf{\Gamma}\mathbf{H}\vec{e}_k], \quad \mathbf{M} = i\mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma},$$

where $i = \sqrt{-1}$, $\mathbf{S} = \mathbf{H} - \Delta^{-1}\partial_t\mathbf{I}$ was defined in (15), and we have defined in (21) $\mathbf{\Gamma} = \mathbf{\Gamma}_\times$ for notational simplicity. Equation (21) follows from applying the integro-differential operator $\vec{\nabla}\Delta^{-1}$ to $\vec{\nabla} \cdot \sigma \vec{E}_k = 0$ in equation (10), with $\vec{E}_k = \vec{\nabla}\chi_k + \vec{e}_k$ and $\sigma = \varepsilon\mathbf{I} + \mathbf{S}$, yielding

$$(22) \quad \mathbf{\Gamma}(\varepsilon\mathbf{I} + \mathbf{S})\vec{\nabla}\chi_k = -\mathbf{\Gamma}\mathbf{H}\vec{e}_k.$$

The equivalence of equations (21) and (22) can be seen by noting that $\vec{\nabla}\chi_k \in \mathcal{H}$ implies $\mathbf{\Gamma}\vec{\nabla}\chi_k = \vec{\nabla}\chi_k$, and writing $1 = -i^2$. We stress that, even though the imaginary unit i was introduced in (21), the representation of $\vec{\nabla}\chi_k$ in this equation is *real-valued*.

In the case of a time-independent velocity field \vec{u} , $\mathbf{S} = \mathbf{H}$ and the operator \mathbf{M} in (21) is given by $\mathbf{M} = i\mathbf{\Gamma}\mathbf{H}\mathbf{\Gamma}$. Recall that $\mathbf{\Gamma}$ is an orthogonal projector from \mathcal{H}_V to \mathcal{H}_\times , and therefore has unit operator norm $\|\mathbf{\Gamma}\| = 1$ on \mathcal{H} [22, 25]. By equation (14), \mathbf{H} is also bounded in operator norm on \mathcal{H} . Therefore, in this time-independent case, \mathbf{M} is a *bounded* linear operator on \mathcal{H} with operator norm $\|\mathbf{M}\| \leq \|\mathbf{\Gamma}\|\|\mathbf{H}\|\|\mathbf{\Gamma}\| = \|\mathbf{H}\| < \infty$. Since \mathbf{M} is bounded, its (Hilbert space) adjoint \mathbf{M}^* is also bounded with $\|\mathbf{M}\| = \|\mathbf{M}^*\|$ [22] and they consequently have common domains,

$$(23) \quad D(\mathbf{M}) = D(\mathbf{M}^*),$$

which are the entire space, $D(\mathbf{M}) = D(\mathbf{M}^*) = \mathcal{H}$. In Section A-1 we show that \mathbf{M} is symmetric

$$(24) \quad \langle \mathbf{M}\vec{\xi} \cdot \vec{\zeta} \rangle = \langle \vec{\xi} \cdot \mathbf{M}\vec{\zeta} \rangle, \quad \text{for all } \vec{\xi}, \vec{\zeta} \in D(\mathbf{M}).$$

By definition [22], the two properties (23) and (24) together imply that the operator \mathbf{M} is *self-adjoint*, i.e. $\mathbf{M} = \mathbf{M}^*$. Conversely, the Hellinger–Toeplitz theorem [22] states that if the operator \mathbf{M} satisfies equation (24) for *every* $\vec{\xi}, \vec{\zeta} \in \mathcal{H}$, then \mathbf{M} is bounded. This suggests that when \mathbf{M} is unbounded on \mathcal{H} , it is defined as a self-adjoint operator only on a proper (dense) subset of \mathcal{H} .

In the case of a time-dependent velocity field \vec{u} , the operator \mathbf{S} is given by $\mathbf{S} = \mathbf{H} - \Delta^{-1}\partial_t\mathbf{I}$. Since \mathcal{V} is a bounded domain, Δ^{-1} is a compact [24], hence bounded operator on \mathcal{H} (more precisely \mathcal{H}_V). The operator $\partial_t\mathbf{I}$, on the other hand, is *unbounded* [22, 25] on \mathcal{H} (more precisely \mathcal{H}_T). Hence \mathbf{M} is unbounded on \mathcal{H} . The unboundedness of $\partial_t\mathbf{I}$ on \mathcal{H} can be seen by considering the orthonormal set of functions $\{\vec{\psi}_n\} \subset \mathcal{H}$ with components $(\vec{\psi}_n)_j$, $j = 1, \dots, d$, defined by

$$(25) \quad (\vec{\psi}_n)_j(t, \vec{x}) = \alpha \sin((n+j)\pi t/T), \quad \alpha = \sqrt{2/(Td)}, \quad \langle \vec{\psi}_n \cdot \vec{\psi}_m \rangle = \delta_{nm}, \quad n, m \in \mathbb{N}.$$

The action of the operator $\partial_t\mathbf{I}$ on the members of the set $\{\vec{\psi}_n\}$ is denoted $\{\partial_t\vec{\psi}_n\}$, and has components $(\partial_t\vec{\psi}_n)_j$ and \mathcal{H} -norm $\|\partial_t\vec{\psi}_n\|$ given by

$$(26) \quad (\partial_t\vec{\psi}_n)_j(t, \vec{x}) = [(n+j)\alpha\pi/T] \cos((n+j)\pi t/T), \quad \|\partial_t\vec{\psi}_n\|^2 = \sum_j [(n+j)\pi/T]^2,$$

which clearly demonstrates the unboundedness of the operator $\partial_t\mathbf{I}$ on \mathcal{H} .

The above analysis demonstrates that the unbounded operator $\mathbf{T} = i\partial_t \mathbf{I}$ is defined only on a proper subset of \mathcal{H} , i.e. $D(\mathbf{T}) \subset \mathcal{H}$. However, the domain $D(\mathbf{T})$ of \mathbf{T} can be defined as a (dense) subset of \mathcal{H} such that \mathbf{T} is bounded [22, 25]. Moreover, on this domain, \mathbf{T} can be extended to a *closed* linear operator [22, 25]. For such a domain, simple integration by parts and the sesquilinearity of the inner-product $\langle \cdot, \cdot \rangle$ shows that, as an operator on $D(\mathbf{T})$, \mathbf{T} is symmetric, i.e. it satisfies (24) with \mathbf{T} in place of \mathbf{M} . Although, in general [22], the domain $D(\mathbf{T}^*)$ of its adjoint \mathbf{T}^* does not satisfy the property displayed in equation (23) and in such circumstances, \mathbf{T} is *not* self-adjoint on $D(\mathbf{T})$. Only for self-adjoint linear operators does the spectral theorem hold [22], which provides the existence of the promised integral representation for κ^* , involving a spectral measure of \mathbf{M} . It is therefore necessary that we find a domain $D(\mathbf{M})$ for which \mathbf{M} is a self-adjoint operator.

Toward this goal, and to illustrate these ideas, we consider the operator $i\partial_t$ with three different domains, which are everywhere dense in $L^2(\mathcal{T})$ [25]. First, consider the set $\hat{\mathcal{D}}_{\mathcal{T}}$ of all functions $\xi \in L^2(\mathcal{T})$ such that $\xi(t)$ is absolutely continuous [23] on the interval \mathcal{T} and has a derivative $\xi'(t)$ belonging to $L^2(\mathcal{T})$, i.e. [25, 23]

$$(27) \quad \hat{\mathcal{D}}_{\mathcal{T}} = \left\{ \xi \in L^2(\mathcal{T}) : \xi(t) = c + \int_0^t g(\tau) d\tau, \quad g \in L^2(\mathcal{T}) \right\},$$

where the constant c and function $g \in L^2(\mathcal{T})$ are arbitrary. Second, consider the set $\tilde{\mathcal{D}}_{\mathcal{T}}$ of all functions $\xi \in \hat{\mathcal{D}}_{\mathcal{T}}$ that satisfy the periodic boundary condition $\xi(0) = \xi(T)$, i.e. functions ξ satisfying the properties of equation (27) with $\int_0^T g(\tau) d\tau = 0$. Finally, consider the set $\mathcal{D}_{\mathcal{T}}$ of all functions $\xi \in \hat{\mathcal{D}}_{\mathcal{T}}$ that satisfy the Dirichlet boundary condition $\xi(0) = \xi(T) = 0$, i.e. functions ξ satisfying the properties of equation (27) with $c = 0$ and $\int_0^T g(\tau) d\tau = 0$. These sets satisfy $\mathcal{D}_{\mathcal{T}} \subset \tilde{\mathcal{D}}_{\mathcal{T}} \subset \hat{\mathcal{D}}_{\mathcal{T}}$ and are each everywhere dense in $L^2(\mathcal{T})$ [25]. Let the operators $\hat{\mathbf{A}}$, $\tilde{\mathbf{A}}$, and \mathbf{A} be identified as $i\partial_t$ with domains $\hat{\mathcal{D}}_{\mathcal{T}}$, $\tilde{\mathcal{D}}_{\mathcal{T}}$, and $\mathcal{D}_{\mathcal{T}}$, respectively. Then [25], \mathbf{A} is a closed, linear, symmetric, operator with adjoint $\mathbf{A}^* \equiv \hat{\mathbf{A}}$, and the operator $\tilde{\mathbf{A}}$ is a *self-adjoint* extension of \mathbf{A} .

Since the set $\tilde{\mathcal{D}}_{\mathcal{T}}$ is everywhere dense in $L^2(\mathcal{T})$ and consists of periodic functions $\xi(t)$ satisfying $\xi(0) = \xi(T)$, the set $\mathcal{A}_{\mathcal{T}} = \otimes_{i=1}^d \tilde{\mathcal{D}}_{\mathcal{T}}$ is everywhere dense in $\mathcal{H}_{\mathcal{T}}$. Moreover, since $\tilde{\mathbf{A}} = i\partial_t$ with domain $\tilde{\mathcal{D}}_{\mathcal{T}}$ is self-adjoint, the operator $\mathbf{T} = i\partial_t \mathbf{I}$ with domain $D(\mathbf{T}) = \mathcal{A}_{\mathcal{T}}$ is self-adjoint. This is seen by noting that, for all $\vec{\xi}, \vec{\zeta} \in \mathcal{A}_{\mathcal{T}}$, $\mathbf{T}\vec{\xi} = (\tilde{\mathbf{A}}\xi_1, \dots, \tilde{\mathbf{A}}\xi_d)$, for example, and

$$(28) \quad \langle \mathbf{T}\vec{\xi} \cdot \vec{\zeta} \rangle = \sum_j \langle \tilde{\mathbf{A}}\xi_j, \zeta_j \rangle_2 = \sum_j \langle \xi_j, \tilde{\mathbf{A}}\zeta_j \rangle_2 = \langle \vec{\xi} \cdot \mathbf{T}\vec{\zeta} \rangle,$$

where $\langle \cdot, \cdot \rangle_2$ denotes the $L^2(\mathcal{T})$ inner-product. It follows that the operator \mathbf{M} defined in equation (21) is self-adjoint on the space $\mathcal{H}_t \subset \mathcal{H}$, which is everywhere dense in \mathcal{H} , given by

$$(29) \quad \mathcal{H}_t = \{ \vec{\xi} \in \mathcal{A}_{\mathcal{T}} \otimes \mathcal{H}_{\times} : \langle \vec{\xi} \rangle = 0 \}.$$

We are now ready to provide an integral representation for the effective diffusivity tensor κ^* . This follows from the spectral theorem of operational calculus in Hilbert space [22, 25], which states that there is a one-to-one correspondence between the self-adjoint operator \mathbf{M} and a family $\{\mathbf{Q}(\lambda)\}$, $-\infty < \lambda < \infty$, of *projection* operators - the resolution of the identity - which satisfies $\lim_{\lambda \rightarrow -\infty} \mathbf{Q}(\lambda) = 0$ and $\lim_{\lambda \rightarrow \infty} \mathbf{Q}(\lambda) = \mathbf{I}$. Moreover, let $\vec{\xi}, \vec{\zeta} \in \mathcal{H}_t$ and consider the following functions $\mu_{\xi\zeta}(\lambda) = \langle \mathbf{Q}(\lambda)\vec{\xi} \cdot \vec{\zeta} \rangle$ and $\mu_{\xi\xi}(\lambda) = \langle \mathbf{Q}(\lambda)\vec{\xi} \cdot \vec{\xi} \rangle = \|\mathbf{Q}(\lambda)\vec{\xi}\|^2$ of *bounded variation* with associated Radon measures $\mu_{\xi\zeta}(d\lambda)$ and $\mu_{\xi\xi}(d\lambda)$ [25]

$$(30) \quad \mu_{\xi\zeta}(d\lambda) = \langle \mathbf{Q}(d\lambda)\vec{\xi} \cdot \vec{\zeta} \rangle, \quad \mu_{\xi\xi}(d\lambda) = \|\mathbf{Q}(d\lambda)\vec{\xi}\|^2.$$

Let $F(\lambda)$ be an arbitrary complex-valued function and denote by $\mathcal{D}(F)$ the set of all $\vec{\xi} \in \mathcal{H}_t$ such that $F \in L^2(\mu_{\xi\xi})$, the class of square $\mu_{\xi\xi}$ -integrable functions. Then $\mathcal{D}(F)$ is a linear manifold and

there exists a linear transformation $\mathbf{M}(F)$ with domain $\mathcal{D}(F)$ defined in terms of the Radon-Stieltjes integral [25]

$$(31) \quad \begin{aligned} \langle \mathbf{M}(F)\vec{\xi} \cdot \vec{\zeta} \rangle &= \int_{-\infty}^{\infty} F(\lambda) \mu_{\xi\zeta}(d\lambda), \quad \forall \vec{\xi} \in \mathcal{D}(F), \vec{\zeta} \in \mathcal{H}_t \\ \langle \mathbf{M}(F)\vec{\xi} \cdot \mathbf{M}(G)\vec{\zeta} \rangle &= \int_{-\infty}^{\infty} F(\lambda)\bar{G}(\lambda) \mu_{\xi\zeta}(d\lambda), \quad \forall \vec{\xi} \in \mathcal{D}(F), \vec{\zeta} \in \mathcal{D}(G), \end{aligned}$$

where \bar{G} denotes the complex conjugate of the function G , the operator $\mathbf{M}(G)$ and set $\mathcal{D}(G)$ involving G and $\vec{\zeta}$ are defined analogously to that for F and $\vec{\xi}$, and the functional $\|\mathbf{M}(F)\vec{\xi}\|^2$ is defined using the second equation in (31) and is defined in terms of a Radon-Stieltjes integral involving the measure $\mu_{\xi\xi}(d\lambda)$ in (30) [25].

An integral representation for the components κ_{jk}^* , $j, k = 1, \dots, d$, of κ^* follows from equations (9) and (21), and the second formula in (31) with

$$(32) \quad F(\lambda) = G(\lambda) = i(-i\varepsilon - \lambda)^{-1}, \quad \vec{\xi} = \vec{g}_j, \quad \vec{\zeta} = \vec{g}_k, \quad \vec{g}_j = \mathbf{\Gamma}\mathbf{H}\vec{e}_j, \quad j, k = 1, \dots, d.$$

More specifically, from equation (14) and the orthogonality of the operators $\mathbf{\Gamma}_\times = \mathbf{\Gamma}$ and $\mathbf{\Gamma}_0$ in (12), the vector $\vec{g}_k = \mathbf{\Gamma}\mathbf{H}\vec{e}_k$ is curl-free, mean-zero, and bounded in \mathcal{H} -norm, i.e. $\vec{g}_k \in \mathcal{H}_t$ with $\|\vec{g}_k\| \leq \|H\|$ for all $k = 1, \dots, d$. Moreover, since $i\varepsilon \in \mathbb{C} \setminus \mathbb{R}$ for all $\varepsilon > 0$ and the measure $\mu_{\xi\xi}(d\lambda)$ is of bounded mass [25]

$$(33) \quad \mu_{\xi\xi}^0 = \int_{-\infty}^{\infty} \mu_{\xi\xi}(d\lambda) = \|\vec{\xi}\|^2 = \langle \mathbf{H}^T \mathbf{\Gamma}\mathbf{H}\vec{g}_k \cdot \vec{g}_k \rangle \leq \|\mathbf{H}\|^2 < \infty,$$

we have that $F(\lambda)$ in (32) satisfies $F \in L^2(\mu_{\xi\xi})$, hence $\vec{g}_j \in \mathcal{D}(F)$, for all $\varepsilon > 0$, $j = 1, \dots, d$. Therefore, the following Radon-Stieltjes integral representation for the components κ_{jk}^* of κ^* , involving the components $\mu_{jk}(d\lambda)$ of the matrix-valued measure $\boldsymbol{\mu}(d\lambda)$, holds for all $\varepsilon > 0$

$$(34) \quad \kappa_{jk}^* = \varepsilon \left(\delta_{jk} + \int_{-\infty}^{\infty} \frac{\mu_{jk}(d\lambda)}{\varepsilon^2 + \lambda^2} \right), \quad \mu_{jk}(d\lambda) = \langle \mathbf{Q}(d\lambda)\vec{g}_j \cdot \vec{g}_k \rangle, \quad j, k = 1, \dots, d.$$

We conclude this section with a few remarks regarding the integral representation in (34). The Radon measure $\mu_{jk}(d\lambda)$ is a *spectral measure* associated with the self-adjoint linear operator \mathbf{M} in the (\vec{g}_j, \vec{g}_k) state [22]. Since $\mathbf{Q}(\lambda)$ is a projection operator, the diagonal components of $\boldsymbol{\mu}(d\lambda)$ are *positive* measures, $\mu_{kk}(d\lambda) = \|\mathbf{Q}(d\lambda)\vec{g}_k\|^2$. In the case of a time-independent velocity field \vec{u} , where $\mathbf{M} = \mathbf{\Gamma}\mathbf{H}\mathbf{\Gamma}$, the range of integration in equation (34) is given by $-\|\mathbf{M}\| \leq \lambda \leq \|\mathbf{M}\|$, with $\|\mathbf{M}\| \leq \|\mathbf{H}\| < \infty$, by (14). In Section 3 we employ the integral representation for κ^* in (34) to obtain asymptotic behavior of κ_{jk}^* as $\varepsilon \rightarrow 0$.

3. ASYMPTOTIC ANALYSIS OF EFFECTIVE DIFFUSIVITY

In two dimensions, $d = 2$, the matrix \mathbf{H} is determined by a stream function $H(t, \vec{x})$

$$(35) \quad \mathbf{H} = \begin{bmatrix} 0 & H \\ -H & 0 \end{bmatrix}, \quad \vec{u} = [\partial_{x_1} H, \partial_{x_2} H].$$

4. NUMERICAL RESULTS

Since we are focusing on flows which are periodic on the spatial region \mathcal{V} , it is convenient to consider the Fourier representation of such a vector field $\vec{\xi}(t, \vec{x})$,

$$(36) \quad \vec{\xi}(t, \vec{x}) = \sum_{\vec{k} \in \mathbb{Z}^d} \hat{Y}(t, \vec{k}) e^{i\vec{k} \cdot \vec{x}}, \quad \hat{Y}(t, \vec{k}) = \frac{1}{(2\pi)^d} \int_{\mathcal{V}} \hat{Y}(t, \vec{x}) e^{-i\vec{k} \cdot \vec{x}} d\vec{x}.$$

The associated action of the above projection operators on a function $\vec{\xi} \in \mathcal{H}$ is given by [8]

$$(37) \quad \begin{aligned} \Gamma_0 \vec{\xi}(t, \vec{x}) &= \langle \vec{\xi}(t, \vec{x}) \rangle_x = \hat{Y}(t, 0), & \Gamma_{\times} \vec{\xi}(t, \vec{x}) &= \sum_{\vec{k} \neq 0} \frac{\vec{k}(\vec{k} \cdot \hat{Y}(t, \vec{k}))}{|\vec{k}|^2} e^{i\vec{k} \cdot \vec{x}}, \\ \Gamma_{\bullet} \vec{\xi}(t, \vec{x}) &= \sum_{\vec{k} \neq 0} \frac{\vec{k} \times (\vec{k} \times \hat{Y}(t, \vec{k}))}{|\vec{k}|^2} e^{i\vec{k} \cdot \vec{x}} = \sum_{\vec{k} \neq 0} \left(I - \frac{\vec{k}\vec{k}}{|\vec{k}|^2} \right) \hat{Y}(t, \vec{k}) e^{i\vec{k} \cdot \vec{x}}, \end{aligned}$$

where $\langle \cdot \rangle_x$ denotes spatial averaging over \mathcal{V} . From equation (37) it is clear that $\Gamma_{\times} + \Gamma_{\bullet} + \Gamma_0 = \mathbf{I}$.

A-1. APPENDIX

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