

SPECTRAL ANALYSIS AND COMPUTATION OF EFFECTIVE DIFFUSIVITIES IN SPACE-TIME PERIODIC FLOWS

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Abstract. The enhancement in diffusive transport of passive tracer particles by incompressible, turbulent flow fields is a challenging problem with theoretical and practical importance in many areas of science and engineering, ranging from the transport of mass, heat, and pollutants in geophysical flows to turbulent combustion and stellar convection. The long time, large scale behavior of such systems is equivalent to an enhanced diffusive process with an effective diffusivity tensor D^* . Based on an analytic continuation method developed for random composite materials, a rigorous integral representation for D^* was developed for the case of a random, *time-independent* fluid velocity field, involving a spectral measure of a self-adjoint random operator acting on *vector-fields*. An alternate approach yielded an integral representation for D^* involving a spectral measure of a self-adjoint operator acting on *scalar-fields*, for the case of a periodic, *time-independent* fluid velocity field. Here, we adapt and extend both of these approaches to the case of a periodic, *time-dependent* fluid velocity field, with possibly chaotic dynamics, providing integral representations for D^* involving spectral measures of the underlying self-adjoint operators. We prove that the two approaches are equivalent and that their correspondence follows from a one-to-one isometry between the underlying Hilbert spaces. We also develop a Fourier method for computing D^* . Our computation in a low dimensional subspace captures the residual diffusion behavior of diffusive transport in time periodic cellular flows with chaotic Lagrangian trajectories.

Key words. advective diffusion, homogenization, effective diffusivity, spectral measure, integral formula, Fourier method, generalized eigenvalue computation, residual diffusion

AMS subject classifications. 47B15, 65C60, 35C15, 76B99 76M22 76M50 76F25 76R99

1. Introduction. The long time, large scale motion of diffusing particles or tracers being advected by an incompressible flow field is equivalent to an enhanced diffusive process [89] with an effective diffusivity tensor D^* . Describing the associated transport properties is a challenging problem with a broad range of scientific and engineering applications, such as stellar convection [48, 77, 19, 20, 18], turbulent combustion [3, 15, 88], and solute transport in porous media [12, 13, 93, 40, 49, 52, 50]. Time-dependent flows can have fluid velocity fields with chaotic dynamics, which gives rise to turbulence that greatly enhances the mixing, dispersion, and large scale transport of diffusing scalars.

In the climate system [24, 39], turbulence plays a key role in transporting mass, heat, momentum, energy, and salt in geophysical flows [65]. Turbulence enhances the dispersion of atmospheric gases [26] such as ozone [42, 74, 75, 76] and pollutants [23, 9, 81], as well as atmosphere-ocean transfers of carbon dioxide and other climatically important trace gas fluxes [95, 7]. Longitudinal dispersion of passive scalars in oceanic flows can be enhanced by horizontal turbulence due to shearing of tidal currents, wind drift, or waves [94, 51, 16]. Chaotic motion of time-dependent fluid velocity fields cause instabilities in large scale ocean currents, generating geostrophic eddies [30] which dominate the kinetic energy of the ocean [31]. Geostrophic eddies greatly enhance [30] the meridional mixing of heat, carbon and other climatically important tracers, typically more than one order of magnitude greater than the mean flow of the ocean [84]. Eddies also impact heat and salt budgets through lateral fluxes and can extend the area of high biological productivity offshore by both eddy chlorophyll advection and eddy nutrient pumping [21]. In sea ice, which couples the atmosphere to the polar oceans [91], the transport of vast ice floes can also be enhanced by eddy fluxes [92, 54].

It has been noted in various geophysical contexts [75, 76] that eddy-induced, skew-diffusive tracer fluxes, directed normal to the tracer gradient [63], are generally equivalent to antisymmetric components in the effective diffusivity tensor D^* , while the symmetric part of D^* represents irreversible diffusive effects [78, 82, 38] directed down the tracer gradient. The mixing of eddy fluxes is typically non-divergent and unable to affect the evolution of the mean flow [63], and do not alter the tracer moments [38]. In this sense, the mixing is non-dissipative, reversible, and sometimes referred to as stirring [25, 38]. Both numerical and observational studies of scalar transport have suggested that tracers are advected over large scales by a fluid velocity field that is different from the mean flow [71]. This suggests that the effective diffusivity tensor D^* should be spatially and possibly also temporally inhomogeneous [71].

Due to the computational intensity of detailed climate models [39, 91, 68], a coarse resolution is necessary in numerical simulations and *parameterization* is used to help resolve sub-grid processes, such as turbulent entrainment-mixing processes in clouds [53], atmospheric boundary layer turbulence [17], atmosphere-surface exchange over the sea [27] and sea ice [83, 1, 2, 90], and eddies in the ocean [59, 36]. In this way, only the

effective or averaged behavior of these sub-grid processes are included in the models. Here, we study the effective behavior of advection enhanced diffusion by time-dependent fluid velocity fields, with possibly chaotic dynamics, which gives rise to such a parameterization, namely, the effective diffusivity tensor D^* of the flow.

In recent decades, a broad range of mathematical techniques have been developed which reduce the analysis of enhanced diffusive transport by complex fluid velocity fields with rapidly varying structures in both space and time, to solving averaged or *homogenized* equations that do not have rapidly varying data, and involve an effective parameter [69, 60, 8, 14, 28, 29, 58, 71, 73, 22, 41, 44, 56, 57]. Motivated by [70], it was shown [60] that the homogenized behavior of the advection-diffusion equation with a random, time-independent, incompressible, mean-zero fluid velocity field, is given by an inhomogeneous diffusion equation involving the symmetric part of an effective diffusivity tensor D^* . Moreover, a rigorous representation of D^* was given in terms of an auxiliary “cell problem” involving a curl-free random field [60]. We stress that the effective diffusivity tensor D^* is not symmetric in general. However, only its symmetric part appears in the homogenized equation for this formulation of the effective transport properties of advection enhanced diffusion [60].

The incompressibility condition of the time-independent fluid velocity field was used [4, 5] to transform the cell problem in [60] into the quasi-static limit of Maxwell’s equations [46, 37], which describe the transport properties of an electromagnetic wave in a composite material [64]. The analytic continuation method for representing transport in composites [37] provides Stieltjes integral representations for the bulk transport coefficients of composite media, such as electrical conductivity and permittivity, magnetic permeability, and thermal conductivity [64]. This method is based on the spectral theorem [87, 79] and a resolvent formula for, say, the electric field, involving a random self-adjoint operator [37, 67] or matrix [66]. Based on [37], the cell problem was transformed into a resolvent formula involving a *bounded* self-adjoint operator, acting on the Hilbert space of curl-free random vector fields [4, 5]. This, in turn, led to a Stieltjes integral representation for the symmetric part of the effective diffusivity tensor D^* , involving the Péclet number Pe of the flow and a *spectral measure* μ of the operator [4, 5]. A key feature of the method is that parameter information in Pe is *separated* from the complicated geometry of the time-independent flow, which is encoded in the measure μ . This property led to rigorous bounds [5] for the diagonal components of D^* . Bounds for D^* can also be obtained using variational methods [5, 28, 29].

The mathematical framework developed in [60] was adapted [71, 61, 56] to the case of a periodic, time-dependent, incompressible fluid velocity field with *non-zero* mean. The velocity field was modeled as a superposition of a large-scale mean flow with small-scale periodically oscillating fluctuations. It was shown [71] that, depending on the strength of the fluctuations relative to the mean flow, the effective diffusivity tensor D^* can be constant or a function of both space and time. When D^* is constant, only its symmetric part appears in the homogenized equation as an enhancement in the diffusivity. However, when D^* is a function of space and time, its antisymmetric part also plays a key role in the homogenized equation. In particular, the symmetric part of D^* appears as an enhancement in the diffusivity, while both the symmetric and antisymmetric parts of D^* contribute to an effective drift in the homogenized equation. The effective drift due to the antisymmetric part is purely sinusoidal, thus divergence-free [71]. This is consistent with what has been observed in geophysical flows in the climate system, as discussed above. In [61], this result was extended to weakly compressible, anelastic fluid velocity fields.

Based on [12], the cell problem discussed in [71] was transformed into a resolvent formula involving a self-adjoint operator, acting on the Sobolev space [62, 32] of spatially periodic scalar fields, which is also a Hilbert space. In the case where the mean flow and periodic fluctuations are time-independent, the self-adjoint operator is compact [12], hence *bounded* [85]. This led to a discrete Stieltjes integral representation for the antisymmetric part of D^* , involving the Péclet number of the steady flow and a spectral measure of the operator.

Here, we generalize both of the approaches described in [4, 5] and [71] to the case of a periodic, *time-dependent* fluid velocity field, allowing for chaotic dynamics. In particular, for each approach, we provide Stieltjes integral representations for both the symmetric and antisymmetric parts of the effective diffusivity tensor D^* , involving a spectral measure of a self-adjoint operator. In this time-dependent setting, the underlying operator becomes *unbounded*. The spectral theory of unbounded operators is more subtle and technically challenging than that of bounded operators. For example, the domain of an unbounded operator and its adjoint plays a central role in the spectral characterization of the operator. Neglecting such

important mathematical details, the Stieltjes integral representation for D^* given in [4, 5] was extended to the time-dependent setting in [6]. Here, we provide a mathematically rigorous formulation of Stieltjes integral representations for D^* in the time-dependent, unbounded operator setting. We prove that the two approaches described in [4, 5] and [71] are equivalent in this setting, and that their correspondence follows from a one-to-one isometry between the underlying Hilbert spaces. We also establish a direct correspondence between the effective parameter problem for D^* and that arising in the analytic continuation method for composite media. Analytical calculations of the spectral measure underlying the effective diffusivity tensor D^* have been obtained only for a handful of simple models of periodic fluid velocity fields to date such as shear flows. We develop a Fourier method for the computation of D^* . In particular, we compute the effective properties for two space dimensional time periodic cellular flows:

$$(1.1) \quad \mathbf{u}(t, \mathbf{x}) = (\cos(y) + \theta \sin(y) \cos(t), \cos(x) + \theta \sin(x) \cos(t)), \quad \theta \in (0, 1], \quad \mathbf{x} = (x, y),$$

whose steady part $(\cos(y), \cos(x))$ is subject to time periodic perturbation that causes transition to Lagrangian chaos [14], [96]. In the advection dominated regime, we shall compare with effective diffusion in steady cellular flows ($\theta = 0$).

The rest of the paper is organized as follows. In section 2, we present homogenization analysis and the integral representation formulas of the effective diffusion tensor in space-time periodic flows. In section 3, we discuss the Fourier method to compute spectral measure and effective diffusion. In section 4, we specialize the Fourier method to (1.1) and derive generalized eigenvalue problems for the spectral measure. In section 5, we show numerical results that illustrate the difference of spectral measures and effective diffusivities in (1.1) when $\theta = 1$ and $\theta = 0$. Proofs of spectral representation formulas of effective diffusivity over vector and scalar fields as well as background materials are in the appendices.

2. Effective transport by advective-diffusion. The density ϕ of a cloud of passive tracer particles diffusing along with molecular diffusivity ε and being advected by an incompressible velocity field \mathbf{u} satisfies the advection-diffusion equation

$$(2.1) \quad \partial_t \phi(t, \mathbf{x}) = \mathbf{u}(t, \mathbf{x}) \cdot \nabla \phi(t, \mathbf{x}) + \varepsilon \Delta \phi(t, \mathbf{x}), \quad \phi(0, \mathbf{x}) = \phi_0(\mathbf{x}),$$

for $t > 0$ and $\mathbf{x} \in \mathbb{R}^d$. Here, the initial density $\phi_0(\mathbf{x})$ and the fluid velocity field \mathbf{u} are assumed given, and \mathbf{u} satisfies $\nabla \cdot \mathbf{u} = 0$. In equation (2.1), $\varepsilon > 0$, d is the spatial dimension of the system, ∂_t denotes partial differentiation with respect to time t , and $\Delta = \nabla \cdot \nabla = \nabla^2$ is the Laplacian. Moreover, $\psi \cdot \varphi = \psi^\dagger \varphi$ and \dagger is the operation of complex-conjugate-transpose, with $\psi \cdot \psi = |\psi|^2$. We stress that all quantities considered in this section are *real-valued*.

We consider enhanced diffusive transport by a periodic fluid velocity field and non-dimensionalize equation (2.1) as follows. Let ℓ and T be typical length and time scales associated with the problem of interest. Mapping to the non-dimensional variables $t \mapsto t/T$ and $\mathbf{x} \mapsto \mathbf{x}/\ell$, one finds that ϕ satisfies the advection-diffusion equation in (2.1) with a non-dimensional molecular diffusivity $\varepsilon \mapsto T\varepsilon/\ell^2$ and velocity field $\mathbf{u} \mapsto T\mathbf{u}/\ell$. There are several different non-dimensionalizations possible for the advection-diffusion equation. A detailed discussion of various non-dimensionalizations involving the Strouhal number, the Péclet number, and the periodic Péclet number is given in [61, 56]. Here, we focus on the long time, large scale transport characteristics of equation (2.1) as a function of ε . To this end, we simply take T to be the temporal periodicity of the velocity field \mathbf{u} and assume that the spatial periodicity of \mathbf{u} is ℓ in all spatial dimensions, i.e.,

$$(2.2) \quad \mathbf{u}(t + T, \mathbf{x}) = \mathbf{u}(t, \mathbf{x}), \quad \mathbf{u}(t, \mathbf{x} + \ell \mathbf{e}_j) = \mathbf{u}(t, \mathbf{x}), \quad j = 1, \dots, d,$$

where \mathbf{e}_j is a standard basis vector in the j th direction.

The long time, large scale dispersion of diffusing tracer particles being advected by an incompressible fluid velocity field is equivalent to an enhanced diffusive process [89] with an effective diffusivity tensor D^* . In recent decades, methods of homogenization theory [60, 28, 56] have been used to provide an explicit representation for D^* . In particular, these methods have demonstrated that the averaged or *homogenized* behavior of the advection-diffusion equation in (2.1), with space-time periodic velocity field \mathbf{u} , is determined by a diffusion equation involving an averaged scalar density $\bar{\phi}$ and an effective diffusivity tensor D^* [56]

$$(2.3) \quad \partial_t \bar{\phi}(t, \mathbf{x}) = \nabla \cdot [D^* \nabla \bar{\phi}(t, \mathbf{x})], \quad \bar{\phi}(0, \mathbf{x}) = \phi_0(\mathbf{x}).$$

Equation (2.3) follows from the assumption that the initial tracer density ϕ_0 varies slowly relative to the variations of the fluid velocity field \mathbf{u} [60, 29, 56]. This information is incorporated into equation (2.1) by introducing a small dimensionless parameter $\delta \ll 1$ and writing [60, 29, 56]

$$(2.4) \quad \phi(0, \mathbf{x}) = \phi_0(\delta \mathbf{x}).$$

Anticipating that ϕ will have diffusive dynamics as $t \rightarrow \infty$, space and time are rescaled according to the standard diffusive relation

$$(2.5) \quad \boldsymbol{\xi} = \mathbf{x}/\delta, \quad \tau = t/\delta^\gamma, \quad \gamma = 2.$$

The rescaled form of equation (2.1) is given by [56]

$$(2.6) \quad \partial_t \phi^\delta(t, \mathbf{x}) = \delta^{-1} \mathbf{u}(t/\delta^2, \mathbf{x}/\delta) \cdot \nabla \phi^\delta(t, \mathbf{x}) + \varepsilon \Delta \phi^\delta(t, \mathbf{x}), \quad \phi(0, \mathbf{x}) = \phi_0(\mathbf{x}),$$

where we have denoted $\phi^\delta(t, \mathbf{x}) = \phi(t/\delta^2, \mathbf{x}/\delta)$. The convergence of ϕ^δ to $\bar{\phi}$ can be rigorously established in the following sense [56]

$$(2.7) \quad \lim_{\delta \rightarrow 0} \sup_{0 \leq t \leq t_0} \sup_{\mathbf{x} \in \mathbb{R}^d} |\phi^\delta(t, \mathbf{x}) - \bar{\phi}(t, \mathbf{x})| = 0,$$

for every finite $t_0 > 0$, provided that ϕ_0 and \mathbf{u} obey some mild smoothness and boundedness conditions, and that \mathbf{u} is *mean-zero*.

For fixed $0 < \delta \ll 1$, an explicit representation of the effective diffusivity tensor \mathbf{D}^* is given in terms of the (unique) mean zero, space-time periodic solution χ_j of the following *cell problem* [14, 56],

$$(2.8) \quad \partial_\tau \chi_j(\tau, \boldsymbol{\xi}) - \varepsilon \Delta_\xi \chi_j(\tau, \boldsymbol{\xi}) - \mathbf{u}(\tau, \boldsymbol{\xi}) \cdot \nabla_\xi \chi_j(\tau, \boldsymbol{\xi}) = u_j(\tau, \boldsymbol{\xi}),$$

where the subscript ξ in Δ_ξ and ∇_ξ indicates that differentiation is with respect to the fast variable $\boldsymbol{\xi}$ defined in equation (2.5). Specifically, the components D_{jk}^* , $j, k = 1, \dots, d$, of the matrix \mathbf{D}^* are given by [60, 28, 56]

$$(2.9) \quad D_{jk}^* = \varepsilon \delta_{jk} + \langle u_j \chi_k \rangle,$$

where δ_{jk} is the Kronecker delta and u_j is the j th component of the vector \mathbf{u} . The averaging $\langle \cdot \rangle$ in (2.9) is with respect to the fast variables defined in equation (2.5). More specifically, consider the bounded sets $\mathcal{T} \subset \mathbb{R}$ and $\mathcal{V} \subset \mathbb{R}^d$, with $\tau \in \mathcal{T}$ and $\boldsymbol{\xi} \in \mathcal{V}$, which define the space-time period cell $((d+1)\text{-torus}) \mathcal{T} \times \mathcal{V}$. In the case of a time-dependent fluid velocity field, $\langle \cdot \rangle$ denotes space-time averaging over $\mathcal{T} \times \mathcal{V}$. In the special case of a time-independent fluid velocity field, the function χ_j is time-independent and satisfies equation (2.8) with $\partial_\tau \chi_j \equiv 0$, and $\langle \cdot \rangle$ in (2.9) denotes spatial averaging over \mathcal{V} [28, 56].

In general, the effective diffusivity tensor \mathbf{D}^* has a symmetric \mathbf{S}^* and antisymmetric \mathbf{A}^* part defined by

$$(2.10) \quad \mathbf{D}^* = \mathbf{S}^* + \mathbf{A}^*, \quad \mathbf{S}^* = \frac{1}{2} (\mathbf{D}^* + [\mathbf{D}^*]^T), \quad \mathbf{A}^* = \frac{1}{2} (\mathbf{D}^* - [\mathbf{D}^*]^T),$$

where $[\mathbf{D}^*]^T$ denotes transposition of the matrix \mathbf{D}^* . Denote by \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* , $j, k = 1, \dots, d$, the components of \mathbf{S}^* and \mathbf{A}^* in (2.10). In Section C.1 we show that they have the following functional representations [71]

$$(2.11) \quad \mathbf{S}_{jk}^* = \varepsilon (\delta_{jk} + \langle \chi_j, \chi_k \rangle_1), \quad \mathbf{A}_{jk}^* = \langle A \chi_j, \chi_k \rangle_1, \quad A = (-\Delta)^{-1} (\partial_t - \mathbf{u} \cdot \nabla),$$

where $\langle f, h \rangle_1 = \langle \nabla f \cdot \nabla h \rangle$ is a Sobolev-type *sesquilinear* inner-product [62] and the operator $(-\Delta)^{-1}$ is based on convolution with respect to the Green's function for the Laplacian Δ [85]. Since the function χ_j is *real-valued* we have $\langle \chi_j, \chi_k \rangle_1 = \langle \chi_k, \chi_j \rangle_1$, which implies that \mathbf{S}^* is a symmetric matrix. The function $A \chi_j$ is also real-valued. We establish in Section C.1 that the operator A is skew-symmetric on a suitable Hilbert space, which implies that $\mathbf{A}_{kj}^* = \langle A \chi_k, \chi_j \rangle_1 = -\langle \chi_k, A \chi_j \rangle_1 = -\langle A \chi_j, \chi_k \rangle_1 = -\mathbf{A}_{jk}^*$ which, in turn, implies that \mathbf{A}^* is an antisymmetric matrix, hence $\mathbf{A}_{kk}^* = \langle A \chi_k, \chi_k \rangle_1 = 0$.

Applying the linear operator $(-\Delta)^{-1}$ to both sides of the cell problem in equation (2.8) yields the following resolvent formula for χ_j

$$(2.12) \quad \chi_j = (\varepsilon + A)^{-1} g_j, \quad g_j = (-\Delta)^{-1} u_j.$$

From equations (2.11) and (2.12) we have the following functional formulas for S_{jk}^* and A_{jk}^* involving the antisymmetric operator A

$$(2.13) \quad S_{jk}^* = \varepsilon (\delta_{jk} + \langle (\varepsilon + A)^{-1} g_j, (\varepsilon + A)^{-1} g_k \rangle_1), \quad A_{jk}^* = \langle A(\varepsilon + A)^{-1} g_j, (\varepsilon + A)^{-1} g_k \rangle_1.$$

Since A is a skew-symmetric operator, it can be written as $A = \iota M$ where M is a symmetric operator. We demonstrate in Section C.1 that M is *self-adjoint* on an appropriate densely defined subset of a Hilbert space.

The spectral theorem for self-adjoint operators states that there is a one-to-one correspondence between the self-adjoint operator M and a family of self-adjoint projection operators $\{Q(\lambda)\}_{\lambda \in \Sigma}$ — the resolution of the identity — that satisfies [87] $\lim_{\lambda \rightarrow \inf \Sigma} Q(\lambda) = 0$ and $\lim_{\lambda \rightarrow \sup \Sigma} Q(\lambda) = I$ [87], where I is the identity operator and Σ is the *spectrum* of M . Define the complex valued function $\mu_{jk}(\lambda) = \langle Q(\lambda) g_j, g_k \rangle_1$, $j, k = 1, \dots, d$, where $g_j = (-\Delta)^{-1} u_j$ is defined in (2.12). Consider the positive measure μ_{kk} and the signed measures $\text{Re } \mu_{jk}$ and $\text{Im } \mu_{jk}$ associated with $\mu_{jk}(\lambda)$, introduced in equation (A.5). Then, given certain regularity conditions on the components u_j of the fluid velocity field \mathbf{u} , for all $0 < \varepsilon < \infty$, the functional formulas for S_{jk}^* and A_{jk}^* in (2.13) have the following Radon–Stieltjes integral representations (see Section C.1 for details)

$$(2.14) \quad S_{jk}^* = \varepsilon \left(\delta_{jk} + \int_{-\infty}^{\infty} \frac{\text{dRe } \mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2} \right), \quad A_{jk}^* = - \int_{-\infty}^{\infty} \frac{\lambda \text{dIm } \mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2}.$$

The periodic homogenization theorem summarized by equations (2.2)–(2.9), as well as its many variations [8, 69, 11, 13, 60, 5, 71, 72, 73, 61, 56], depend on the detailed nature of the fluid velocity field \mathbf{u} . They also depend on the temporal scaling used [13, 71, 56], i.e., what value of γ is used in equation (2.5). However, the mathematical structure of the cell problem in (2.8) and the functional form of D^* displayed in equation (2.9) remain unchanged for the space-time periodic setting. One of the key goals of the present work is to develop a rigorous mathematical framework that provides Stieltjes integral representations for effective diffusivity tensor D^* for *time-dependent* \mathbf{u} , involving a spectral measure of a self-adjoint operator acting on an appropriate Hilbert space. We will demonstrate that this mathematical framework depends only on the structure of the cell problem in (2.8) and the presence of an inner-product in the functional form of D^* in (2.9). In particular, the theoretical development is insensitive to the detailed nature of \mathbf{u} and depends only on its boundedness properties (See Corollary C.2 for details). Consequently, our results given here apply in many of the well studied systems and will likely apply to many of the homogenization results of the future.

In order to illustrate the rich behaviors that can arise in the effective diffusivity tensor D^* for more general velocity fields and alternate temporal scalings, we now briefly discuss some key variations of the theory described above. When the fluid velocity field is mean-zero, as discussed above, then equation (2.7) holds and the effective diffusivity tensor D^* defined in (2.9) is constant [56]. Consequently, only the symmetric part of D^* plays a role in the effective transport equation displayed in (2.3). Now consider a more general fluid velocity field

$$(2.15) \quad \mathbf{u}(t, \mathbf{x}) = \delta^\alpha \mathbf{u}_0(\delta^\gamma t, \delta \mathbf{x}) + \mathbf{u}_1(t, \mathbf{x}), \quad \alpha = 1, \quad \gamma = 2,$$

which is the superposition of a *weak*, large-scale mean flow $\delta \mathbf{u}_0(\delta^2 t, \delta \mathbf{x})$ that varies on large spatial and slow time scales, with a mean-zero periodic flow $\mathbf{u}_1(t, \mathbf{x})$ that rapidly fluctuates in space and time [56]. If $\mathbf{u}_0(t, \mathbf{x})$ is smooth and bounded, the homogenization theorem for purely periodic velocity fields discussed above can be rigorously extended to the present setting and the effective transport equation in (2.3) is replaced by [56]

$$(2.16) \quad \partial_t \bar{\phi}(t, \mathbf{x}) = \mathbf{u}_0(t, \mathbf{x}) \cdot \nabla \bar{\phi}(t, \mathbf{x}) + \nabla \cdot [D^* \nabla \bar{\phi}(t, \mathbf{x})], \quad \bar{\phi}(0, \mathbf{x}) = \phi_0(\mathbf{x}),$$

which includes an advective enhancement in transport by the large-scale mean flow \mathbf{u}_0 [56]. In this case, the effective diffusivity tensor D^* is completely independent of the mean flow \mathbf{u}_0 , and is determined by the same formula in equation (2.9) and the same cell problem in (2.8) with $\mathbf{u} \rightarrow \mathbf{u}_1$ [56]. Consequently, D^* is again constant and only the symmetric part of D^* plays a role in the effective transport equation displayed in (2.16).

This problem was studied in [71] for scalings in (2.15) different than $\alpha = 1$ and $\gamma = 2$. The parameter α determines the strength of the mean flow \mathbf{u}_0 relative to the small scale periodic fluctuations \mathbf{u}_1 . When

the mean flow is weak compared to the fluctuations, to leading order, \mathbf{D}^* is constant and independent of the mean flow, which only determines the transport velocity on large length and long time scales. Consequently, only the symmetric part of \mathbf{D}^* plays a role in the effective transport equation, which is similar to that in (2.16) [71]. Regardless of the values of α and γ , in the weak mean flow regime, the components D_{jk}^* of the effective diffusivity tensor are given by a formula analogous to equation (2.9) and the structure of the cell problem is analogous to equation (2.8). There are three distinct behaviors that arise as the values of α and γ vary, and the function χ_j in (2.8) can be time-dependent or time-independent ($\partial_\tau \chi_j \equiv 0$) [71].

As we discussed in Section 1, the constancy of the effective diffusivity tensor \mathbf{D}^* is not consistent with measurements and numerical simulations of passive tracer transport in the ocean and atmosphere. However, when the fluid velocity is active on both the slow and fast time scales, with $\gamma = 1$, and the mean flow is equal in strength or stronger than the periodic fluctuations, then \mathbf{D}^* *is a function of space and time* [71]. Consequently, in the effective transport equation, the *antisymmetric* part of \mathbf{D}^* contributes to a purely rotational (divergence-free) enhancement in advective transport, while the symmetric part of \mathbf{D}^* contributes to an enhancement in advective and diffusive transport [71]. This is consistent with observations and direct numerical simulations of geophysical flows in the climate system.

In Section C.1 we provide a mathematically rigorous formulation of Stieltjes integral representations for both the symmetric and antisymmetric parts of the effective diffusivity tensor \mathbf{D}^* . This formulation is based on the spectral theorem for *unbounded* self-adjoint operators in Hilbert space, which is based on an axiomatic construction of Hilbert space. Consequently, the integral representations for \mathbf{D}^* depend only on abstract properties of the underlying self-adjoint operator and, in particular, on boundedness properties shared by a large class of fluid velocity fields \mathbf{u} , including all those discussed in this section. In Section A, we review the spectral theory of unbounded operators, which arise naturally in the study of advection enhanced diffusive transport by time-dependent periodic flows. In Section C we give two natural Hilbert space formulations of the effective parameter problem for \mathbf{D}^* which lead to its promised integral representations. In Section F.2 we use powerful methods of functional analysis to prove that the two formulations are equivalent and discuss the theoretical and computational advantages of each approach.

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3. Cell flows and Fourier methods. In this section we discuss how Fourier methods can be employed to calculate the symmetric \mathbf{D}^* and anti-symmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* for a large class of velocity fields \mathbf{u} . It is more natural to focus on the approach discussed in Section ??, as opposed to that of Section F.1, as the underlying operators are *sparse* (infinite) matrices in Fourier space and the velocity field \mathbf{u} appears naturally, as opposed to the stream matrix \mathbf{H} . Our use of Fourier methods in this section is two-fold. In Section 3.1, we will apply them to the eigenvalue problem $A\varphi_n = \imath\lambda_n\varphi_n$ to explicitly calculate the discrete component of the spectral measure $d\mu(\lambda)$ underlying the integral representations for \mathbf{D}^* and \mathbf{A}^* displayed in equation (F.43).

3.1. Spectral methods. In this section, we use Fourier and spectral methods in concert to obtain explicit representations for the spectral weights $\langle\varphi_n, g_j\rangle_1 \langle\varphi_n, g_k\rangle_1$, $n \in \mathbb{Z}$, $j, k = 1, \dots, d$, at the heart of the integral representations for \mathbf{D}^* and \mathbf{A}^* , displayed in equation (F.43), for a large class of velocity fields \mathbf{u} . In particular, we consider velocity fields \mathbf{u} with components u_j , $j = 1, \dots, d$, which are representable by a *finite* number of Fourier modes. More specifically, we consider $\mathbf{u} \in \mathcal{U}$, where

$$(3.1) \quad \mathcal{U} = \otimes_{j=1}^d \mathcal{U}_j, \quad \mathcal{U}_j = \left\{ u_j \in \mathcal{H}^1 : u_j = \sum_{(\ell, \mathbf{k}) \in I_M^{d+1}} b_{\ell, \mathbf{k}}^j e^{\imath(\ell t + \mathbf{k} \cdot \mathbf{x})} \right\}, \quad b_{\ell, \mathbf{k}}^j = \langle u_j(t, \mathbf{x}), e^{\imath(\ell t + \mathbf{k} \cdot \mathbf{x})} \rangle_2,$$

where \mathcal{H}^1 is defined in equation (F.31), $\mathbf{k} = (k_1, \dots, k_d)$, and the summation index set I_M^{d+1} is defined as $I_M^{d+1} = \{\mathbf{q} \in \mathbb{Z}^{d+1} : -M \leq q_i \leq M, M \in \mathbb{N}\}$. It is well known that \mathcal{U} is dense in \mathcal{H}^1 [33].

Consider the eigenvalue problem $A\varphi_n = \imath\lambda_n\varphi_n$, $\lambda_n \in \mathbb{R}$, $n \in \mathbb{Z}$, involving the integro-differential operator $A = \Delta^{-1}(\mathbf{u} \cdot \nabla - \partial_t)$ defined in equation (2.11). This equation may be rewritten as

$$(3.2) \quad (\mathbf{u} \cdot \nabla - \partial_t)\varphi_n = \imath\lambda_n\Delta\varphi_n.$$

Since $\varphi_n \in \mathcal{F} \subset \mathcal{H}^1$ and $\{e^{\imath(\ell t + \mathbf{k} \cdot \mathbf{x})} : \ell \in \mathbb{Z}, \mathbf{k} \in \mathbb{Z}^d\}$ is an orthonormal basis in \mathcal{H}^1 [33] we may represent φ_n by

$$(3.3) \quad \varphi_n(t, \mathbf{x}) = \sum_{(\ell, \mathbf{k}) \in \mathbb{Z}^{d+1}} a_{\ell, \mathbf{k}}^n e^{\imath(\ell t + \mathbf{k} \cdot \mathbf{x})},$$

Inserting this into equation (3.2) and denoting $\mathbf{b}_{\ell', \mathbf{k}'} = (b_{\ell', \mathbf{k}'}^1, \dots, b_{\ell', \mathbf{k}'}^d)$ the Fourier coefficients of $\mathbf{u} = (u_1, \dots, u_d)$ in (3.1) yields

$$(3.4) \quad \sum_{(\ell, \mathbf{k}) \in \mathbb{Z}^{d+1}} a_{\ell, \mathbf{k}}^n e^{\imath(\ell t + \mathbf{k} \cdot \mathbf{x})} \left(\sum_{(\ell', \mathbf{k}') \in I_M^{d+1}} e^{\imath(\ell' t + \mathbf{k}' \cdot \mathbf{x})} [\mathbf{b}_{\ell', \mathbf{k}'} \cdot \imath \mathbf{k}] - \imath \ell + \imath \lambda_n |\mathbf{k}|^2 \right) = 0.$$

Combining, removing the common factor \imath , and renumbering the summation involving $e^{\imath((\ell + \ell')t + (\mathbf{k} + \mathbf{k}') \cdot \mathbf{x})}$ in (3.4) yields,

$$(3.5) \quad \sum_{(\ell, \mathbf{k}) \in \mathbb{Z}^{d+1}} e^{\imath(\ell t + \mathbf{k} \cdot \mathbf{x})} \left(\sum_{(\ell', \mathbf{k}') \in I_M^{d+1}} [\mathbf{b}_{\ell', \mathbf{k}'} \cdot (\mathbf{k} - \mathbf{k}')] a_{\ell - \ell', \mathbf{k} - \mathbf{k}'}^n - \ell a_{\ell, \mathbf{k}}^n + \lambda_n |\mathbf{k}|^2 a_{\ell, \mathbf{k}}^n \right) = 0.$$

Since the orthogonal set $\{e^{\imath(\ell t + \mathbf{k} \cdot \mathbf{x})} : \ell \in \mathbb{Z}, \mathbf{k} \in \mathbb{Z}^d\}$ is complete, we have [87, 47] from (3.5) that

$$(3.6) \quad \sum_{(\ell', \mathbf{k}') \in I_M^{d+1}} [\mathbf{b}_{\ell', \mathbf{k}'} \cdot (\mathbf{k} - \mathbf{k}')] a_{\ell - \ell', \mathbf{k} - \mathbf{k}'}^n - \ell a_{\ell, \mathbf{k}}^n = -\lambda_n |\mathbf{k}|^2 a_{\ell, \mathbf{k}}^n.$$

Equation (3.6) defines a matrix equation as follows. Define the bijective linear mapping Θ of I_M^{d+1} to $I_M = \{q \in \mathbb{Z} : 1 \leq q_i \leq (2M + 1)^d, M \in \mathbb{N}\}$, $\Theta : I_M^d \mapsto I_M$,

$$(3.7) \quad \Theta(\ell, \mathbf{k}) = 1 + \sum_{j=1}^d (M + k_j)(2M + 1)^{j-1} + (M + \ell)(2M + 1)^d.$$

We now discuss how the $L^2(\mathcal{T} \times \mathcal{V})$ trigonometric orthogonality relation

$$(3.8) \quad \left\langle e^{i(\ell t + \mathbf{k} \cdot \mathbf{x})}, e^{i(\ell' t + \mathbf{k}' \cdot \mathbf{x})} \right\rangle_2 = \delta_{\ell, \ell'} \prod_{j=1}^d \delta_{k_j, k'_j}$$

provides a convenient series representation for the spectral weights $\overline{\langle \varphi_n, g_j \rangle_1} \langle \varphi_n, g_k \rangle_1$ underlying the integral representations for \mathbf{D}^* and \mathbf{A}^* displayed in equation (F.43). This representation follows from equations (F.47), (3.3), and (3.8)

$$(3.9) \quad \langle \varphi_n, g_j \rangle_1 = \langle \varphi_n, u_j \rangle_2 = \sum_{(\ell', \mathbf{k}') \in I_M^{d+1}} \overline{a_{\ell', \mathbf{k}'}^n} b_{\ell', \mathbf{k}'}^j$$

We now discuss how the orthogonality condition $\langle \varphi_n, \varphi_i \rangle_1 = \delta_{li}$ in (F.32) is transformed by the Fourier expansion of the eigenfunctions $\varphi_n(t, \mathbf{x})$. This expansion of $\varphi_n(t, \mathbf{x})$ implies that for $\nabla \varphi_n(t, \mathbf{x})$ as follows

$$(3.10) \quad \varphi_n(t, \mathbf{x}) = \sum_{\ell, m, n} a_{\ell, m, n}^l e^{i(\ell t + m x + n y)} \Rightarrow \nabla \varphi_n(t, \mathbf{x}) = \sum_{\ell, m, n} a_{\ell, m, n}^l (m, n) e^{i(\ell t + m x + n y)}.$$

where $\langle \cdot, \cdot \rangle_2$ denotes the $L^2(\mathcal{T} \times \mathcal{V})$ -inner-product, and that $\langle \cdot \rangle$ denotes space-time averaging. Consequently, we have that the orthogonality relation in (F.32) is transformed to

$$(3.11) \quad \delta_{li} = \langle \nabla \varphi_n \cdot \nabla \varphi_i \rangle = \sum_{\ell, m, n} (m^2 + n^2) \overline{a_{\ell, m, n}^l} a_{\ell, m, n}^i$$

Recall that $\sum_i i^{-p}$ converges for all $p > 1$. From this and equation (3.11) we see that the square modulus of the Fourier coefficients $a_{\ell, m, n}^l$ must have the asymptotic behavior $|a_{\ell, m, n}^l|^2 \sim o((m^2 + n^2)^{-3/2})$ as $m, n \rightarrow \pm\infty$. Since $\varphi_n(\cdot, \mathbf{x}) \in \tilde{\mathcal{A}}_T(\mathcal{T})$, i.e. $\partial_t \varphi_n(\cdot, \mathbf{x}) \in L^2(\mathcal{T})$, we also have $|a_{\ell, m, n}^l|^2 \sim o(\ell^{-3})$ as $\ell \rightarrow \pm\infty$. Since $\partial_t \nabla \varphi_n \in L^2(\mathcal{T} \times \mathcal{V})$ we may generalize both of these statements by the following

$$(3.12) \quad |a_{\ell, m, n}^l|^2 \sim o(\ell^{-3}(m^2 + n^2)^{-3/2}), \text{ as } \ell, m, n \rightarrow \pm\infty.$$

4. Numerical Results. Consider the eigenvalue problem $A\varphi_n = i\lambda_n\varphi_n$, $i = \sqrt{-1}$, $\lambda_n \in \mathbb{R}$, $l = 1, 2, 3, \dots$, involving the integro-differential operator $A = (-\Delta)^{-1}(\partial_t + \mathbf{u} \cdot \nabla)$, introduced in equation (45) of our (attached) effective-diffusivity paper, with $\mathbf{u} \mapsto -\mathbf{u}$. Here A is an anti-symmetric (normal) operator and the incompressible velocity field $\mathbf{u}(t, \mathbf{x})$ is given in equation (4.13) above. The equation $A\varphi_n = i\lambda_n\varphi_n$ may be rewritten as

$$(4.1) \quad (\partial_t + \mathbf{u} \cdot \nabla)\varphi_n = -i\lambda_n\Delta\varphi_n.$$

The eigenfunctions φ_n satisfy the following orthogonality condition in (F.32)

The eigenfunction φ_n is $\mathcal{T} \times \mathcal{V}$ periodic, mean-zero, and $\varphi_n \in \tilde{\mathcal{A}}_T(\mathcal{T}) \otimes \mathcal{H}^1(\mathcal{V})$, i.e. it is absolutely continuous in time for $t \in \mathcal{T}$, and is in the Sobolev space $\mathcal{H}^1(\mathcal{V})$ for $\mathbf{x} \in \mathcal{V}$. We denote the class of such functions by \mathcal{F}

$$(4.2) \quad \mathcal{F} = \{f \in \tilde{\mathcal{A}}_T(\mathcal{T}) \otimes \mathcal{H}^1(\mathcal{V}) \mid \langle f \rangle = 0 \text{ and is periodic on } \mathcal{T} \times \mathcal{V}\}.$$

Since the orthogonal set $\{e^{i\ell t}\}$, $\ell \in \mathbb{Z}$, is dense in $\tilde{\mathcal{A}}_T(\mathcal{T})$, we may represent φ_n by

$$(4.3) \quad \varphi_n(t, \mathbf{x}) = \sum_{\ell} \varphi_{\ell}^l(\mathbf{x}) e^{i\ell t},$$

where $\varphi_{\ell}^l \in \mathcal{H}^1(\mathcal{V})$. Write $\cos t = (e^{it} + e^{-it})/2$ and insert this and (4.3) into equation (4.1), yielding

$$(4.4) \quad \sum_{\ell} (i\ell + \mathbf{u}_1 \cdot \nabla + i\lambda_n\Delta)\varphi_{\ell}^l(\mathbf{x})e^{i\ell t} + \frac{\delta}{2} \sum_{\ell} (e^{i(\ell+1)t} + e^{i(\ell-1)t}) \mathbf{u}_2 \cdot \nabla \varphi_{\ell}^l(\mathbf{x}) = 0,$$

or:

$$(4.5) \quad \sum_{\ell} \left[(\imath \ell + \mathbf{u}_1 \cdot \nabla + \imath \lambda_n \Delta) \varphi_{\ell}^l(\mathbf{x}) + \frac{\delta}{2} \mathbf{u}_2 \cdot \nabla (\varphi_{\ell-1}^l(\mathbf{x}) + \varphi_{\ell+1}^l(\mathbf{x})) \right] e^{\imath \ell t} = 0.$$

By the completeness in $L^2(\mathcal{T})$ of the orthogonal set $\{e^{\imath \ell t}\}$ we have, for each $\ell \in \mathbb{Z}$,

$$(4.6) \quad (\imath \ell + \mathbf{u}_1 \cdot \nabla) \varphi_{\ell}^l(\mathbf{x}) + \frac{\delta}{2} \mathbf{u}_2 \cdot \nabla (\varphi_{\ell-1}^l(\mathbf{x}) + \varphi_{\ell+1}^l(\mathbf{x})) = -\imath \lambda_n \Delta \varphi_{\ell}^l(\mathbf{x}).$$

The system of partial differential equations in (4.6) can be reduced to a system of algebraic equations as follows. Recall that $\mathbf{u}_1(\mathbf{x}) = (\cos y, \cos x)$ and $\mathbf{u}_2(\mathbf{x}) = (\sin y, \sin x)$, which implies

$$(4.7) \quad \begin{aligned} (\mathbf{u}_1 \cdot \nabla) \varphi_{\ell}^l(\mathbf{x}) &= \cos y \partial_x \varphi_{\ell}^l(\mathbf{x}) + \cos x \partial_y \varphi_{\ell}^l(\mathbf{x}) \\ (\mathbf{u}_2 \cdot \nabla) \varphi_{\ell}^l(\mathbf{x}) &= \sin y \partial_x \varphi_{\ell}^l(\mathbf{x}) + \sin x \partial_y \varphi_{\ell}^l(\mathbf{x}) \end{aligned}$$

Since $\varphi_{\ell}^l \in \mathcal{H}^1(\mathcal{V})$ and the orthogonal set $\{e^{\imath(mx+ny)}\}$, $m, n \in \mathbb{Z}$, is dense in this space, we can represent $\varphi_{\ell}^l(\mathbf{x})$ by

$$(4.8) \quad \varphi_{\ell}^l(\mathbf{x}) = \sum_{m,n} a_{\ell,m,n}^l e^{\imath(mx+ny)}$$

Write $\cos x = (e^{\imath x} + e^{-\imath x})/2$ and $\sin x = (e^{\imath x} - e^{-\imath x})/(2\imath)$, for example, and insert this and (4.8) into equation (4.7), yielding

$$(4.9) \quad \begin{aligned} (\mathbf{u}_1 \cdot \nabla) \varphi_{\ell}^l &= \frac{1}{2} \sum_{m,n} a_{\ell,m,n}^l \left[\imath m e^{\imath m x} (e^{\imath(n+1)y} + e^{\imath(n-1)y}) + \imath n e^{\imath n y} (e^{\imath(m+1)x} + e^{\imath(m-1)x}) \right] \\ (\mathbf{u}_2 \cdot \nabla) \varphi_{\ell}^l &= \frac{1}{2\imath} \sum_{m,n} a_{\ell,m,n}^l \left[\imath m e^{\imath m x} (e^{\imath(n+1)y} - e^{\imath(n-1)y}) + \imath n e^{\imath n y} (e^{\imath(m+1)x} - e^{\imath(m-1)x}) \right] \end{aligned}$$

or:

$$(4.10) \quad \begin{aligned} (\mathbf{u}_1 \cdot \nabla) \varphi_{\ell}^l &= \frac{\imath}{2} \sum_{m,n} [m(a_{\ell,m,n-1}^l + a_{\ell,m,n+1}^l) + n(a_{\ell,m-1,n}^l + a_{\ell,m+1,n}^l)] e^{\imath(mx+ny)} \\ (\mathbf{u}_2 \cdot \nabla) \varphi_{\ell}^l &= \frac{1}{2} \sum_{m,n} [m(a_{\ell,m,n-1}^l - a_{\ell,m,n+1}^l) + n(a_{\ell,m-1,n}^l - a_{\ell,m+1,n}^l)] e^{\imath(mx+ny)}. \end{aligned}$$

We also have

$$(4.11) \quad -\Delta \varphi_{\ell}^l = \sum_{m,n} a_{\ell,m,n}^l (m^2 + n^2) e^{\imath(mx+ny)}$$

By the completeness of the orthogonal set $\{e^{\imath(mx+ny)}\}$, inserting equations (4.10) and (4.11) into equation (4.6) yields

$$(4.12) \quad \begin{aligned} \imath \ell a_{\ell,m,n}^l &+ \frac{\imath}{2} [m(a_{\ell,m,n-1}^l + a_{\ell,m,n+1}^l) + n(a_{\ell,m-1,n}^l + a_{\ell,m+1,n}^l)] \\ &+ \frac{\delta}{4} [m(a_{\ell-1,m,n-1}^l - a_{\ell-1,m,n+1}^l) + n(a_{\ell-1,m-1,n}^l - a_{\ell-1,m+1,n}^l) \\ &+ m(a_{\ell+1,m,n-1}^l - a_{\ell+1,m,n+1}^l) + n(a_{\ell+1,m-1,n}^l - a_{\ell+1,m+1,n}^l)] \\ &= \imath \lambda_n (m^2 + n^2) a_{\ell,m,n}^l, \end{aligned}$$

which is an infinite system of algebraic equations for the unknown Fourier coefficients $a_{\ell,m,n}^l$ associated with the eigenfunctions $\varphi_n(t, \mathbf{x})$ and eigenvalues $\imath \lambda_n$, $l \in \mathbb{N}$ and $\ell, m, n \in \mathbb{Z}$. Recalling that φ_n is mean-zero $\langle \varphi_n \rangle = 0$, we have that $\ell^2 + m^2 + n^2 > 0$.

We now show that the special nature of the velocity field in (4.13) and the Fourier expansion of the eigenfunctions φ_n in (3.10) allow the spectral weights $\langle \varphi_n, g_j \rangle$ in equation (F.43) to be given in terms of the Fourier coefficients $a_{\ell,m,n}^l$ for the reduced index set $\ell, m, n \in \{-1, 0, 1\}$.

$$(4.13) \quad \mathbf{u}(t, \mathbf{x}) = (\cos y, \cos x) + \delta \cos t (\sin y, \sin x) := \mathbf{u}_1(\mathbf{x}) + \delta \cos t \mathbf{u}_2(\mathbf{x}).$$

Writing $\cos x = (e^{ix} + e^{-ix})/2$ and $\sin x = (e^{ix} - e^{-ix})/(2i)$, for example, from equation (4.13) we have that

$$(4.14) \quad \begin{aligned} u_1(t, x, y) &= \cos y + \cos t \sin y \\ &= \frac{1}{2} (e^{iy} + e^{-iy}) + \frac{1}{4i} (e^{it} + e^{-it})(e^{iy} - e^{-iy}) \\ &= \frac{1}{2} (e^{iy} + e^{-iy}) + \frac{1}{4i} \left(e^{i(t+y)} - e^{i(t-y)} + e^{i(-t+y)} - e^{i(-t-y)} \right), \end{aligned}$$

and $u_2(t, x, y) = u_1(t, y, x)$. This, equation (F.47), and the orthogonality relation in (3.8) imply that

$$(4.15) \quad \begin{aligned} \langle \varphi_n, g_1 \rangle_1 &= \frac{1}{2} (a_{0,0,1}^l + a_{0,0,-1}^l) + \frac{1}{4i} (a_{1,0,1}^l - a_{1,0,-1}^l + a_{-1,0,1}^l - a_{-1,0,-1}^l) \\ \langle \varphi_n, g_2 \rangle_1 &= \frac{1}{2} (a_{0,1,0}^l + a_{0,-1,0}^l) + \frac{1}{4i} (a_{1,1,0}^l - a_{1,-1,0}^l + a_{-1,1,0}^l - a_{-1,-1,0}^l) \end{aligned}$$

Since \mathbf{u}_i is incompressible, there exists an anti-symmetric matrix \mathbf{H}_i such that $\mathbf{u}_i = \nabla \cdot \mathbf{H}_i$. This allows us to write $\mathbf{u}_i \cdot \nabla = \nabla \cdot \mathbf{H}_i \nabla$, which is an anti-symmetric operator. When $\delta = 0$, the velocity field \mathbf{u} is time-independent and the operator A , which arises from the cell problem, becomes $A = (-\Delta)^{-1}(\mathbf{u}_1 \cdot \nabla)$. In this case, the eigenvalue problem in (4.1) becomes

$$(4.16) \quad \nabla \cdot \mathbf{H}_1 \nabla \varphi = \lambda \Delta \varphi.$$

Discretizing this equation leads to a generalized eigenvalue problem involving *sparse* matrices. This matrix formulation has all the desired properties of the associated abstract Hilbert space formulation. (I will be adding the details of this to our paper soon.) From this matrix problem, we obtain a discrete approximation of the Radon–Stieltjes integral representation for the symmetric \mathbf{D}^* and anti-symmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* , displayed in equation (35) of our (attached) paper.

4.1. Matrix representations of the eigenvalue problem. In the *time-independent case*, where $\delta = 0$ in the velocity field of equation (4.13), the system of equations in (4.12) corresponding to the eigenvalue problem becomes

$$(4.17) \quad m(a_{m,n-1} + a_{m,n+1}) + n(a_{m-1,n} + a_{m+1,n}) = 2\lambda(m^2 + n^2)a_{m,n}, \quad m, n \in \mathbb{Z},$$

where, for simplicity, we have dropped the super-script and sub-script, and have written $a_{m,n} = a_{m,n}^l$ and $\lambda = \lambda_n$. When the indices in equation (4.17) are restricted to be finite, $-M \leq m, n \leq M$ say, and suitable boundary conditions are imposed, it can be written in matrix form

$$(4.18) \quad B\mathbf{a}_l = 2\lambda_n C\mathbf{a}_l,$$

where B and C are $(2M+1)^2 \times (2M+1)^2$ symmetric matrices and $l = 1, \dots, (2M+1)^2$. More specifically, B is real-symmetric and C is real-diagonal positive-semi-definite. Equation (4.18) is a generalized eigenvalue problem. Since B and C are symmetric matrices, the generalized eigenvalues are real $\lambda_n \in \mathbb{R}$ and the eigen-vectors \mathbf{a}_l – consisting of the Fourier coefficients for φ_n – satisfy the orthogonality condition

$$(4.19) \quad \mathbf{a}_j^T C \mathbf{a}_k = \delta_{jk}.$$

The rows and columns of B and C , corresponding to the $a_{0,0}$ component of \mathbf{a} , consist entirely of zero elements. Therefore, without loss of generality, they can be removed from these matrices, making the matrix C positive-definite.

FIG. 1. *Caption*

In the *time-dependent* case, where $\delta \neq 0$ in the velocity field of equation (4.13), slightly manipulating equation (4.12) yields

$$\begin{aligned}
 & 4\ell a_{\ell,m,n} + 2[m(a_{\ell,m,n-1} + a_{\ell,m,n+1}) + n(a_{\ell,m-1,n} + a_{\ell,m+1,n})] \\
 & - i\delta[m(a_{\ell-1,m,n-1} - a_{\ell-1,m,n+1} + a_{\ell+1,m,n-1} - a_{\ell+1,m,n+1}) \\
 & + n(a_{\ell-1,m-1,n} - a_{\ell-1,m+1,n} + a_{\ell+1,m-1,n} - a_{\ell+1,m+1,n})] \\
 & = 4\lambda(m^2 + n^2)a_{\ell,m,n}.
 \end{aligned}
 \tag{4.20}$$

By restricting the indices, $-M \leq l, m, n \leq M$, in equation (4.20) and imposing suitable boundary conditions, it can also be written as the generalized eigenvalue problem of equations (4.18) and (4.19), where B and C are $(2M+1)^3 \times (2M+1)^3$ symmetric matrices. More specifically, B is Hermitian-symmetric and C is real-diagonal. The rows and columns of B and C , corresponding to the $a_{0,0,0}$ component of \mathbf{a} , consist entirely of zero elements. Therefore, without loss of generality, they can be removed from the generalized eigenvalue problem, making the matrix C positive-definite.

5. Numerical Results. In this section we discuss the numerical implementation of the integral representations in equation (??), involving the signed, discrete measures displayed in (??). In particular, we directly compute the spectral measure $d\mu(\lambda)$ associated with discretizations of velocity fields \mathbf{u} for model flows, to compute the symmetric D^* and anti-symmetric A^* parts of the associated effective diffusivity tensor D^* . We explore the numerical implementation of the different formulations of the effective parameter

problem, described by Corollary ?? and Theorem C.1 which involve the anti-symmetric operators A and \mathbf{A} , respectively. This analysis demonstrates that formulation described by Corollary ?? provides a more practical numerical implementation than that described in Theorem C.1, as A is a *sparse* matrix of size N , say, and \mathbf{A} is a *full* matrix of size dN .

Appendix A. Spectral theory of unbounded self-adjoint operators in Hilbert space. The theory of *unbounded* (linear) operators in Hilbert space was developed largely by John von Neumann and Marshall H. Stone. It is considerably more technical and challenging than that of bounded operators, as unbounded operators do not form an algebra, nor even a linear space, because each one is defined on its own domain. In this section, we review the spectral theory for such operators and, in particular, the celebrated *spectral theorem* for self-adjoint operators [79, 87].

Let Φ be a linear operator acting on a Hilbert space \mathcal{H} with sesquilinear inner-product $\langle \cdot, \cdot \rangle$ satisfying $\langle a\psi, b\varphi \rangle = a\bar{b}\langle \psi, \varphi \rangle$ and $\langle \psi, \varphi \rangle = \overline{\langle \varphi, \psi \rangle}$ for all $\psi, \varphi \in \mathcal{H}$ and $a, b \in \mathbb{C}$, where \bar{z} denotes complex conjugation of $z \in \mathbb{C}$. The \mathcal{H} -inner-product induces a norm $\|\cdot\|$ defined by $\|\psi\| = \langle \psi, \psi \rangle^{1/2}$. The (Hilbert space) adjoint Φ^* of Φ is defined by $\langle \Phi\psi, \varphi \rangle = \langle \psi, \Phi^*\varphi \rangle$. If Φ is *bounded* in operator norm, i.e., $\|\Phi\| = \sup_{\{\psi \in \mathcal{H} : \|\psi\|=1\}} \|\Phi\psi\| < \infty$, then $\|\Phi^*\| = \|\Phi\|$ [79]. Consequently, Φ and its adjoint Φ^* have identical domains,

$$(A.1) \quad D(\Phi) = D(\Phi^*),$$

as they can be taken, without loss of generality [85], to be the entire Hilbert space, $D(\Phi) = D(\Phi^*) = \mathcal{H}$. The operator Φ is said to be *symmetric* if [79]

$$(A.2) \quad \langle \Phi\psi, \varphi \rangle = \langle \psi, \Phi\varphi \rangle, \text{ for all } \psi, \varphi \in D(\Phi).$$

By definition [79, 87], the two properties (A.1) and (A.2) together imply that the operator Φ is *self-adjoint*, i.e. $\Phi \equiv \Phi^*$ on $D(\Phi)$.

Conversely, the Hellinger–Toeplitz theorem states, if the operator Φ satisfies $\langle \Phi\psi, \varphi \rangle = \langle \psi, \Phi\varphi \rangle$ for *every* $\psi, \varphi \in \mathcal{H}$, then Φ is bounded on \mathcal{H} [79]. This suggests that, if Φ is *unbounded* on \mathcal{H} , then it is defined as a self-adjoint operator only on a proper subset of \mathcal{H} . However, the domain $D(\Phi)$ can sometimes be defined as an *everywhere dense* subset of \mathcal{H} such that Φ is bounded. On this domain, the symmetric operator Φ can be extended to a *closed* symmetric operator [79, 87]. However, even in this case the domain of Φ does not always coincide with $D(\Phi^*)$, and in such circumstances Φ is *not* self-adjoint. A self-adjoint operator is a maximal symmetric operator, meaning that it has no proper symmetric extensions [87]. Only for self-adjoint operators does the spectral theorem hold [79, 87].

The spectrum Σ of a self-adjoint operator Φ on a Hilbert space \mathcal{H} is real-valued [79, 87]. If Φ is bounded, then its spectral radius equal to its operator norm $\|\Phi\|$ [79], i.e.,

$$(A.3) \quad \Sigma \subseteq [-\|\Phi\|, \|\Phi\|].$$

If Φ is unbounded, its spectrum Σ can be an unbounded subset of, or can even coincide with the set of real numbers \mathbb{R} [87].

We now summarize the spectral theorem for self-adjoint operators [87]. Let Φ be a self-adjoint operator with densely defined domain $D(\Phi) \subset \mathcal{H}$. If Φ is bounded then we simply take $D(\Phi) \equiv \mathcal{H}$. The spectral theorem states that there is a one-to-one correspondence between the self-adjoint operator Φ and a family of self-adjoint projection operators $\{Q(\lambda)\}_{\lambda \in \Sigma}$ — the resolution of the identity — that satisfies [87]

$$(A.4) \quad \lim_{\lambda \rightarrow \inf \Sigma} Q(\lambda) = 0, \quad \lim_{\lambda \rightarrow \sup \Sigma} Q(\lambda) = I,$$

where 0 and I denote the null and identity operators on \mathcal{H} , respectively. Furthermore, the *complex-valued* function of the spectral variable λ defined by $\mu_{\psi\varphi}(\lambda) = \langle Q(\lambda)\psi, \varphi \rangle$ is strictly increasing for $\lambda \in \Sigma$ and of bounded variation for all $\psi, \varphi \in D(\Phi)$ [87].

By the sesquilinearity of the inner-product and the self-adjointness of the projection operator $Q(\lambda)$, the function $\mu_{\psi\varphi}(\lambda)$ satisfies $\mu_{\varphi\psi}(\lambda) = \overline{\mu_{\psi\varphi}(\lambda)}$. Moreover, the function $\mu_{\psi\psi}(\lambda)$ is real-valued and positive $\mu_{\psi\psi}(\lambda) = \langle Q(\lambda)\psi, \psi \rangle = \langle Q(\lambda)\psi, Q(\lambda)\psi \rangle = \|Q(\lambda)\psi\|^2 \geq 0$. Consider the associated real-valued functions

$$(A.5) \quad \text{Re } \mu_{\psi\varphi}(\lambda) = \frac{1}{2} (\mu_{\psi\varphi}(\lambda) + \overline{\mu_{\psi\varphi}(\lambda)}), \quad \text{Im } \mu_{\psi\varphi}(\lambda) = \frac{1}{2i} (\mu_{\psi\varphi}(\lambda) - \overline{\mu_{\psi\varphi}(\lambda)}),$$

where $\iota = \sqrt{-1}$, $\text{Re } \mu_{\psi\psi}(\lambda) = \mu_{\psi\psi}(\lambda)$ and $\text{Im } \mu_{\psi\psi}(\lambda) = 0$. With each of these strictly increasing functions of bounded variation, we associate Stieltjes measures [86, 87, 33]

$$(A.6) \quad \begin{aligned} d\mu_{\psi\varphi}(\lambda) &= d\langle Q(\lambda)\psi, \varphi \rangle, & d\text{Re } \mu_{\psi\varphi}(\lambda) &= d\text{Re } \langle Q(\lambda)\psi, \varphi \rangle, \\ d\mu_{\psi\psi}(\lambda) &= d\|Q(\lambda)\psi\|^2, & d\text{Im } \mu_{\psi\varphi}(\lambda) &= d\text{Im } \langle Q(\lambda)\psi, \varphi \rangle, \end{aligned}$$

which we will denote by $\mu_{\psi\psi}$, $\mu_{\psi\varphi}$, $\text{Re } \mu_{\psi\varphi}$, and $\text{Im } \mu_{\psi\varphi}$. We stress that $\mu_{\psi\psi}$ is a positive measure, $\mu_{\psi\varphi}$ is a complex measure, while $\text{Re } \mu_{\psi\varphi}$ and $\text{Im } \mu_{\psi\varphi}$ are signed measures [86, 87].

The spectral theorem also provides an operational calculus in Hilbert space which yields powerful integral representations involving the Stieltjes measures displayed in equation (A.6). A summary of the relevant details are as follows. Let $F(\lambda)$ and $G(\lambda)$ be arbitrary complex-valued functions and denote by $\mathcal{D}(F)$ the set of all $\psi \in D(\Phi)$ such that $F \in L^2(\mu_{\psi\psi})$, i.e., F is square integrable on the set Σ with respect to the *positive* measure $\mu_{\psi\psi}$, and similarly define $\mathcal{D}(G)$. Then $\mathcal{D}(F)$ and $\mathcal{D}(G)$ are linear manifolds and there exists linear operators denoted by $F(\Phi)$ and $G(\Phi)$ with domains $\mathcal{D}(F)$ and $\mathcal{D}(G)$, respectively, which are defined in terms of the following Radon–Stieltjes integrals [87]

$$(A.7) \quad \begin{aligned} \langle F(\Phi)\psi, \varphi \rangle &= \int_{-\infty}^{\infty} F(\lambda) d\mu_{\psi\varphi}(\lambda), & \forall \psi \in \mathcal{D}(F), \varphi \in D(\Phi), \\ \langle F(\Phi)\psi, G(\Phi)\varphi \rangle &= \int_{-\infty}^{\infty} F(\lambda) \overline{G(\lambda)} d\mu_{\psi\varphi}(\lambda), & \forall \psi \in \mathcal{D}(F), \varphi \in \mathcal{D}(G), \end{aligned}$$

where the integration in (A.7) is over the spectrum Σ of Φ [79, 87].

The mass $\mu_{\psi\varphi}^0 = \int_{-\infty}^{\infty} d\mu_{\psi\varphi}(\lambda)$ of the Stieltjes measure $\mu_{\psi\varphi}$ satisfies [87] $\mu_{\psi\varphi}^0 = \lim_{\lambda \rightarrow \sup \Sigma} \mu_{\psi\varphi}(\lambda) - \lim_{\lambda \rightarrow \inf \Sigma} \mu_{\psi\varphi}(\lambda)$. Consequently, equation (A.4) yields

$$(A.8) \quad \mu_{\psi\varphi}^0 = \int_{-\infty}^{\infty} d\langle Q(\lambda)\psi, \varphi \rangle = \langle \psi, \varphi \rangle, \quad |\mu_{\psi\varphi}^0| \leq \|\psi\| \|\varphi\| < \infty.$$

Equation (A.8) demonstrates that the measures in (A.6) are *finite measures*, i.e., they have bounded mass [87].

Equation (A.7) can be generalized, holding with suitable notational changes, for *maximal normal operators* [87]. Such a normal operator \mathbf{N} with densely defined domain $D(\mathbf{N}) \subset \mathcal{H}$ commutes with its adjoint \mathbf{N}^* , i.e., $\mathbf{N}\mathbf{N}^* = \mathbf{N}^*\mathbf{N}$, and can be decomposed as $\mathbf{N} = \Phi_1 + \iota\Phi_2$, where Φ_1 and Φ_2 are self-adjoint and commute. The spectrum of the normal operator \mathbf{N} is a (possibly unbounded) subset of \mathbb{C} [87]. A special case of a normal operator is a *skew-adjoint* operator satisfying $\mathbf{N}^* = -\mathbf{N}$. It can be decomposed as $\mathbf{N} = \iota\Phi_2$ and since Φ_2 is self-adjoint having purely real spectrum, the skew-adjoint operator $\mathbf{N} = \iota\Phi_2$ has purely imaginary spectrum [87]. Consequently, given such a maximal skew-adjoint operator, one can focus attention on the self-adjoint operator $\Phi_2 = -\iota\mathbf{N}$ without having to resort to the more notationally complicated spectral theory of normal operators.

The signed measures $\text{Re } \mu_{\psi\varphi}$ and $\text{Im } \mu_{\psi\varphi}$ displayed in equation (A.6) arise naturally when considering a maximal skew-adjoint operator $\mathbf{N} = \iota\Phi$, where Φ is self-adjoint. This can be illustrated by considering some special cases. Consider the functional $\langle F(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle$ involving *real-valued* Hilbert space members $F(\mathbf{N})\psi$ and $G(\mathbf{N})\varphi$, so that $\langle F(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle = \langle G(\mathbf{N})\varphi, F(\mathbf{N})\psi \rangle \in \mathbb{R}$ and, in particular,

$$(A.9) \quad \langle F(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle = \frac{1}{2} (\langle F(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle + \langle G(\mathbf{N})\varphi, F(\mathbf{N})\psi \rangle).$$

Now consider the special cases $F(\mathbf{N}) = G(\mathbf{N})$ and $F(\mathbf{N}) = \mathbf{N}G(\mathbf{N})$, i.e., $F(\iota\lambda) = G(\iota\lambda)$ and $F(\iota\lambda) = \iota\lambda G(\iota\lambda)$ in equation (A.7), respectively. It follows from equations (A.7) and (A.9), the identities $\text{Re } z = (z + \bar{z})/2$ and $\text{Im } z = (z - \bar{z})/(2\iota)$, and the linearity properties [87] of Stieltjes–Radon integrals with respect to the functions $\mu_{\psi\varphi}(\lambda)$ and $\bar{\mu}_{\psi\varphi}(\lambda)$ that

$$(A.10) \quad \begin{aligned} \langle G(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle &= \int_{-\infty}^{\infty} |G(\iota\lambda)|^2 d\text{Re } \mu_{\psi\varphi}(\lambda), \\ \langle \mathbf{N}G(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle &= - \int_{-\infty}^{\infty} \lambda |G(\iota\lambda)|^2 d\text{Im } \mu_{\psi\varphi}(\lambda). \end{aligned}$$

An important property of a self-adjoint operator Φ which will be used later is that its domain $D(\Phi)$ comprises those and only those elements $\psi \in \mathcal{H}$ such that the Stieltjes integral $\int_{-\infty}^{\infty} \lambda^2 d\mu_{\psi\psi}(\lambda)$ is convergent. When $\psi \in D(\Phi)$ the element $\Phi\psi$ is determined by the relations [87]

$$(A.11) \quad \langle \Phi\psi, \varphi \rangle = \int_{-\infty}^{\infty} \lambda d\mu_{\psi\varphi}(\lambda), \quad \|\Phi\psi\|^2 = \int_{-\infty}^{\infty} \lambda^2 d\mu_{\psi\psi}(\lambda),$$

where φ is an arbitrary element in $D(\Phi)$ [87]. In fact, this determines the one-to-one correspondence between the self-adjoint operator Φ and its resolution of the identity $Q(\lambda)$ [87].

Appendix B. The time derivative as a maximal normal operator. A key example of an unbounded operator is the time derivative ∂_t acting on the space $L^2(\mathcal{T})$ of Lebesgue measurable functions that are also square integrable on the interval $\mathcal{T} = [0, T]$, say. The unboundedness of ∂_t as an operator on $L^2(\mathcal{T})$ can be understood by considering the orthonormal set of functions $\{\varphi_n\} \subset L^2(\mathcal{T})$ defined by

$$(B.1) \quad \varphi_n(t) = \beta \sin(n\pi t/T), \quad \beta = \sqrt{2/T}, \quad \langle \varphi_n, \varphi_m \rangle_2 = \delta_{nm}, \quad n, m \in \mathbb{N},$$

where $\langle \cdot, \cdot \rangle_2$ denotes the sesquilinear $L^2(\mathcal{T})$ -inner-product. It follows from $\partial_t \varphi_n = (n\pi\beta/T) \cos(n\pi t/T)$ and $\|\partial_t \varphi_n\|^2 = (n\pi/T)^2$, that the norm of the members of the set $\{\partial_t \varphi_n\}$ grows arbitrarily large as $n \rightarrow \infty$. This clearly demonstrates the unboundedness of the operator ∂_t with domain $L^2(\mathcal{T})$.

When one also imposes periodic or Dirichlet boundary conditions, simple integration by parts demonstrates that the operator ∂_t is *skew-symmetric* on $L^2(\mathcal{T})$ so that $-i\partial_t$ is symmetric with respect to the sesquilinear inner-product $\langle \cdot, \cdot \rangle_2$. We now identify an everywhere dense subset of $L^2(\mathcal{T})$ on which $-i\partial_t$ is a bounded linear self-adjoint operator [79, 87]. Consider the class $\mathcal{A}_{\mathcal{T}}$ of all functions $\psi \in L^2(\mathcal{T})$ such that $\psi(t)$ is *absolutely continuous* [80] on the interval \mathcal{T} and has a derivative $\psi'(t)$ belonging to $L^2(\mathcal{T})$, i.e., [87, 80]

$$(B.2) \quad \mathcal{A}_{\mathcal{T}} = \left\{ \psi \in L^2(\mathcal{T}) \mid \psi(t) = c + \int_0^t g(s)ds, \quad g \in L^2(\mathcal{T}) \right\},$$

where the constant c and function $g(s)$ are arbitrary. Now, consider the set $\tilde{\mathcal{A}}_{\mathcal{T}}$ of all functions $\psi \in \mathcal{A}_{\mathcal{T}}$ that satisfy the periodic boundary condition $\psi(0) = \psi(T)$, i.e. functions ψ satisfying the properties of equation (B.2) with $\int_0^T g(s)ds = 0$. In order to help clarify the ideas that were discussed in Section A in terms of an abstract Hilbert space \mathcal{H} , we also consider the set $\hat{\mathcal{A}}_{\mathcal{T}}$ of all functions $\psi \in \mathcal{A}_{\mathcal{T}}$ that satisfy the Dirichlet boundary condition $\psi(0) = \psi(T) = 0$, i.e. functions ψ satisfying the properties of equation (B.2) with $c = 0$ and $\int_0^T g(s)ds = 0$. More concisely,

$$(B.3) \quad \tilde{\mathcal{A}}_{\mathcal{T}} = \{\psi \in \mathcal{A}_{\mathcal{T}} \mid \psi(0) = \psi(T)\}, \quad \hat{\mathcal{A}}_{\mathcal{T}} = \{\psi \in \mathcal{A}_{\mathcal{T}} \mid \psi(0) = \psi(T) = 0\}.$$

These function spaces satisfy $\hat{\mathcal{A}}_{\mathcal{T}} \subset \tilde{\mathcal{A}}_{\mathcal{T}} \subset \mathcal{A}_{\mathcal{T}}$ and are each everywhere dense in $L^2(\mathcal{T})$ [87]. Let the operators B , \tilde{B} , and \hat{B} be identified as $-i\partial_t$ with domains $\mathcal{A}_{\mathcal{T}}$, $\tilde{\mathcal{A}}_{\mathcal{T}}$, and $\hat{\mathcal{A}}_{\mathcal{T}}$, respectively. Then, \hat{B} is a closed linear symmetric operator with the adjoint $\hat{B}^* \equiv B$, and the operator \tilde{B} is a *self-adjoint* extension of \hat{B} [87]. In symbols, this means that $\tilde{B} = \tilde{B}^*$ on $\tilde{\mathcal{A}}_{\mathcal{T}}$ and $D(\tilde{B}) = D(\tilde{B}^*) = \tilde{\mathcal{A}}_{\mathcal{T}}$, i.e., $\tilde{B} \equiv \tilde{B}^*$ on $\tilde{\mathcal{A}}_{\mathcal{T}}$. This establishes that the operator $-i\partial_t$ with domain $\tilde{\mathcal{A}}_{\mathcal{T}}$ is self-adjoint, hence ∂_t is a maximal skew-symmetric (normal) operator on $\tilde{\mathcal{A}}_{\mathcal{T}}$. The operator $i\partial_t$ on $\mathcal{A}_{\mathcal{T}}$ has a simple point spectrum, consisting of eigenvalues $\lambda = 2n\pi/T$, $n \in \mathbb{Z}$, with corresponding eigenfunctions $\exp(2n\pi t/T)$ [87].

Appendix C. Hilbert spaces, resolvents, and integral representations of the effective diffusivity. In this section we formulate a spectral theory of effective diffusivities for space-time periodic flows. In Section C.1 we address an approach suggested in [71], while in Section C.2 we address an approach suggested in [6]. In each case, we provide a rigorous mathematical framework which leads to Stieltjes integral representations for both the symmetric S^* and antisymmetric A^* parts of the effective diffusivity tensor D^* for space-time periodic flows, involving a spectral measure of an *unbounded* self-adjoint operator. In Section F.2 we use the one-to-one correspondence between a self-adjoint operator and its resolution of the identity [87], discussed in the paragraph containing equation (A.11), to establish that the two approaches are equivalent.

C.1. Scalar fields and the effective diffusivity. In this section we provide an abstract Hilbert space formulation of the effective parameter problem for advection enhanced diffusion by a space-time periodic fluid velocity field $\mathbf{u}(t, \mathbf{x})$. Consider the following sets $\mathcal{T} = [0, T]$ and $\mathcal{V} = \times_{j=1}^d [0, \ell]$ which define the space-time period cell $\mathcal{T} \times \mathcal{V}$ for $\mathbf{u}(t, \mathbf{x})$. Now consider the Hilbert spaces $L^2(\mathcal{T})$ and $L^2(\mathcal{V})$ of Lebesgue measurable functions over the complex field \mathbb{C} that are also square integrable on \mathcal{T} and \mathcal{V} , respectively. Define the associated Hilbert spaces $\mathcal{H}_{\mathcal{T}}$ and $\mathcal{H}_{\mathcal{V}}$,

$$(C.1) \quad \mathcal{H}_{\mathcal{T}} = \{\psi \in L^2(\mathcal{T}) \mid \psi(t) = \psi(t+T)\}, \quad \mathcal{H}_{\mathcal{V}} = \{\psi \in L^2(\mathcal{V}) \mid \psi(\mathbf{x}) = \psi(\mathbf{x} + \ell \mathbf{e}_j)\},$$

for all $j = 1, \dots, d$, where the \mathbf{e}_j are standard basis vectors. Denote by $\langle \cdot \rangle$ space-time averaging over $\mathcal{T} \times \mathcal{V}$. Now define the Hilbert space $\mathcal{H}_{\mathcal{T}\mathcal{V}} = \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$ with sesquilinear inner-product $\langle \cdot, \cdot \rangle$ given by $\langle \psi, \varphi \rangle = \langle \psi \varphi \rangle$, with $\langle \varphi, \psi \rangle = \overline{\langle \psi, \varphi \rangle}$. The $\mathcal{H}_{\mathcal{T}\mathcal{V}}$ -inner-product induces a norm $\| \cdot \|$ given by $\| \psi \| = \langle \psi, \psi \rangle^{1/2}$ [33].

In equation (B.3) we defined the space $\mathcal{A}_{\mathcal{T}}$ of absolutely continuous \mathcal{T} -periodic functions with derivatives belonging to $\mathcal{H}_{\mathcal{T}}$, which is an everywhere dense subset of the Hilbert space $\mathcal{H}_{\mathcal{T}}$ [87]. We now define the Sobolev space $\mathcal{H}_{\mathcal{V}}^1$, which is also a Hilbert space [12, 32, 62],

$$(C.2) \quad \mathcal{H}_{\mathcal{V}}^1 = \{\psi \in \mathcal{H}_{\mathcal{V}} \mid \langle |\nabla \psi|^2 \rangle_{\mathcal{V}} < \infty\},$$

where $\langle \cdot \rangle_{\mathcal{V}}$ denotes spatial averaging over \mathcal{V} . Finally, consider the Hilbert space \mathcal{H} and its everywhere dense subset \mathcal{F} defined by

$$(C.3) \quad \mathcal{H} = \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1, \quad \mathcal{F} = \mathcal{A}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1.$$

Recalling that $\psi \cdot \varphi = \psi^\dagger \varphi$, the sesquilinear \mathcal{H} -inner-product is given by $\langle \psi, \varphi \rangle_1 = \langle \nabla \psi \cdot \nabla \varphi \rangle$ with associated norm $\| \cdot \|_1$ given by $\| \psi \|_1 = \langle |\nabla \psi|^2 \rangle^{1/2}$. We stress that $\psi \in \mathcal{F}$ implies $\| \partial_t \psi \|_1 < \infty$ and $\| \psi \|_1 < \infty$. In the case of a time-independent fluid velocity field $\mathbf{u}(\mathbf{x})$ we set $\mathcal{H} \equiv \mathcal{F} \equiv \mathcal{H}_{\mathcal{V}}^1$.

We now use properties of the Hilbert space \mathcal{H} to obtain functional formulas for the symmetric \mathbf{S}^* and antisymmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* defined in equations (2.9) and (2.10), involving the solution χ_j of the cell problem in equation (2.8) and a maximal skew-symmetric operator A on \mathcal{F} . We then transform the cell problem into a resolvent formula for χ_j involving the operator A . The spectral theorem discussed in Section A then yields the promised Stieltjes integral representations for \mathbf{S}^* and \mathbf{A}^* . We will henceforth assume that $u_j, \chi_j \in \mathcal{F}$ for all $j = 1, \dots, d$.

Applying the linear operator $(-\Delta)^{-1}$ to both sides of the cell problem in equation (2.8) yields

$$(C.4) \quad (-\Delta)^{-1} u_j = (\varepsilon + A) \chi_j,$$

where we have defined $A = (-\Delta)^{-1}(\partial_t - \mathbf{u} \cdot \nabla)$. The operator $(-\Delta)^{-1}$ is based on convolution with respect to the Green's function for the Laplacian Δ and is bounded on $L^2(\mathcal{V})$ [85], hence $\mathcal{H}_{\mathcal{V}}^1$. Now write the functional $\langle u_j \chi_k \rangle$ in equation (2.9) as [71]

$$(C.5) \quad \langle u_j \chi_k \rangle = \langle [\Delta \Delta^{-1} u_j] \chi_k \rangle = -\langle \nabla \Delta^{-1} u_j \cdot \nabla \chi_k \rangle = \langle (-\Delta)^{-1} u_j, \chi_k \rangle_1.$$

This calculation will be rigorously justified in Theorem C.1 below. Substituting the formula for $(-\Delta)^{-1} u_j$ in (C.4) into equation (C.5) yields equation (2.11), which provides functional formulas for the components \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* , $j, k = 1, \dots, d$, of \mathbf{S}^* and \mathbf{A}^* . Equation (C.4) is equivalent to the the resolvent formula displayed in equation (2.12). From equations (2.11) and (2.12) we have the functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* displayed in equation (2.13), involving the operator A . The following theorem establishes the promised Stieltjes integral representations for the functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* in (2.13).

THEOREM C.1. *The operator $A = (-\Delta)^{-1}(\partial_t - \mathbf{u} \cdot \nabla)$ displayed in equation (2.11) is a maximal (skew-symmetric) normal operator on the function space \mathcal{F} defined in equation (C.3), hence $M = -\imath A$ is a self-adjoint operator on \mathcal{F} . Let $Q(\lambda)$ be the resolution of the identity in one-to-one correspondence with M . Define the complex valued function $\mu_{jk}(\lambda) = \langle Q(\lambda) g_j, g_k \rangle_1$, $j, k = 1, \dots, d$, where $g_j = (-\Delta)^{-1} u_j$ is defined in (2.12) and $\langle \cdot, \cdot \rangle_1$ is the \mathcal{H} -inner-product. Consider the positive measure μ_{kk} and the signed measures $\text{Re} \mu_{jk}$ and $\text{Im} \mu_{jk}$ associated with $\mu_{jk}(\lambda)$, introduced in equation (A.5). Then, for $u_j, \chi_j \in \mathcal{F}$ and all $0 < \varepsilon < \infty$, the functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* displayed in (2.13) have the Radon-Stieltjes integral representations displayed in equation (2.14).*

Proof of Theorem C.1. We first establish that $M = -\iota A$ is a self-adjoint operator on \mathcal{F} . The Sobelov space \mathcal{H}_V^1 in (C.2) is the closure in the norm $\langle |\nabla \psi|^2 \rangle_V$ of the space of all twice continuously differentiable periodic functions in \mathcal{H}_V , and all the elements of \mathcal{H}_V^1 are those elements of \mathcal{H}_V which have square integrable gradients on the set V [12]. Furthermore, the elements of $\tilde{\mathcal{A}}_T$ are those elements of \mathcal{H}_T that are differentiable almost everywhere (except on a set of Lebesgue measure zero), have square integrable derivatives on the interval T , and are indefinite integrals of their derivative, hence continuous [80]. Consequently, $f \in \mathcal{F}$ implies that $(-\Delta)^{-1} \partial_t f = \partial_t (-\Delta)^{-1} f$ [33, 85] and [87, 80]

$$(C.6) \quad \|f\|_\infty = \sup_{(t, \mathbf{x}) \in T \times V} |f(t, \mathbf{x})| < \infty,$$

For $u_j \in \mathcal{F}$ and fixed $t \in T$, equation (C.6) implies that $[\mathbf{u}(t, \cdot) \cdot \nabla] : \mathcal{H}_V^1 \rightarrow \mathcal{H}_V$, while $(-\Delta)^{-1} : \mathcal{H}_V \rightarrow \mathcal{H}_V^1$ [12]. In particular, for $f, h \in \mathcal{F}$ we have that $\langle (-\Delta)^{-1} f, h \rangle_1 = \langle f, h \rangle$ [12]. This justifies the calculation in equation (C.5).

We have already established in Section B that the operator $-\iota \partial_t$ is self-adjoint on $\tilde{\mathcal{A}}_T$ [87]. The integral operator $(-\Delta)^{-1}$ is self-adjoint and compact on \mathcal{H}_V [85]. Since they commute on \mathcal{F} , it follows that the operator $-\iota (-\Delta)^{-1} \partial_t$ is self-adjoint on \mathcal{F} , hence $(-\Delta)^{-1} \partial_t$ is a maximal (skew-symmetric) normal operator on \mathcal{F} [87].

We now establish that the operator $(-\Delta)^{-1} [\mathbf{u} \cdot \nabla]$ is antisymmetric and compact on \mathcal{F} . The antisymmetry of this operator depends on the incompressibility, $\nabla \cdot \mathbf{u} = 0$, of the fluid velocity field and was established in [12, 71]. Since the operator $(-\Delta)^{-1}$ is compact on \mathcal{H}_V [85], we need only show that the operator $\mathbf{u} \cdot \nabla$ is bounded on \mathcal{F} . This is established by the following calculation. For $u_j, f \in \mathcal{F}$, equation (C.6) yields

$$(C.7) \quad \begin{aligned} \|\mathbf{u} \cdot \nabla f\|^2 &= |\langle \mathbf{u} \cdot \nabla f, \mathbf{u} \cdot \nabla f \rangle| \\ &\leq \sum_{jk} |\langle u_j \partial_j f, u_k \partial_k f \rangle| \quad (\text{triangle inequality}) \\ &\leq \max_j \|u_j\|_\infty^2 \sum_{jk} |\langle \partial_j f, \partial_k f \rangle| \\ &\leq \max_j \|u_j\|_\infty^2 \sum_{jk} \|\partial_j f\| \|\partial_k f\| \quad (\text{Cauchy-Schwartz}) \\ &= \max_j \|u_j\|_\infty^2 \left[\sum_j \|\partial_j f\| \right]^2 \\ &\leq d \max_j \|u_j\|_\infty^2 \sum_j \|\partial_j f\|^2 \quad (\text{Cauchy-Schwartz}) \\ &= d \max_j \|u_j\|_\infty^2 \|f\|_1^2. \end{aligned}$$

This demonstrates that the operator norm $\|\mathbf{u} \cdot \nabla\|$ has the upper bounded $\|\mathbf{u} \cdot \nabla\| \leq \sqrt{d} \max_j \|u_j\|_\infty$ and establishes that $(-\Delta)^{-1} [\mathbf{u} \cdot \nabla]$ is a compact operator on \mathcal{F} . Since the operator $(-\Delta)^{-1} [\mathbf{u} \cdot \nabla]$ is antisymmetric and compact, hence *bounded* on \mathcal{F} , it is a maximal (skew-adjoint) normal operator on \mathcal{F} , hence $-\iota (-\Delta)^{-1} [\mathbf{u} \cdot \nabla]$ is self-adjoint on \mathcal{F} [87].

Denote $M = -\iota A$, where $A = (-\Delta)^{-1} (\partial_t - \mathbf{u} \cdot \nabla)$. Since A is a linear operator, we have established that M is self-adjoint on \mathcal{F} . Since the operator $(-\Delta)^{-1} [\mathbf{u} \cdot \nabla]$ is bounded on \mathcal{F} we can take the domain $D(M)$ of M to be $D(M) = \mathcal{F}$. The complex-valued functions involved in the functional formulas for S_{jk}^* and A_{jk}^* in equation (2.13) are $F(\lambda) = (\varepsilon + \iota \lambda)^{-1}$ and $G(\lambda) = \iota \lambda (\varepsilon + \iota \lambda)^{-1}$. For all $0 < \varepsilon < \infty$, we have $|F(\lambda)|^2 = (\varepsilon^2 + \lambda^2)^{-1} \leq \varepsilon^{-2} < \infty$ and $|G(\lambda)|^2 = \lambda^2 (\varepsilon^2 + \lambda^2)^{-1} \leq 1$. Since μ_{kk} is a finite measure for all $k = 1, \dots, d$, as shown in equation (A.8), we therefore have that $f \in \mathcal{D}(F)$ and $f \in \mathcal{D}(G)$ for all $f \in D(M)$ when $0 < \varepsilon < \infty$. Since $u_j \in \mathcal{F}$ and $(-\Delta)^{-1}$ is a bounded operator on \mathcal{F} , we have that $g_j = (-\Delta)^{-1} u_j \in \mathcal{F}$. The conditions of the spectral theorem are thus satisfied. Consequently, the integral representations in equation (A.7) hold for the functions $F(\lambda)$ and $G(\lambda)$ defined above, involving the complex measure μ_{jk} . The discussion leading to equation (A.10) then establishes the integral representations for S_{jk}^* and A_{jk}^* displayed in equation (2.14). This completes the proof of Theorem C.1 \square .

We conclude this section with a discussion regarding an extension of Theorem C.1 to a broader class of fluid velocity fields, summarized by the following corollary.

COROLLARY C.2. *Theorem C.1 can be extended to the following class \mathcal{U} of fluid velocity fields \mathbf{u} , having components u_j , $j = 1, \dots, d$,*

$$(C.8) \quad \mathcal{U} = \{u_j \in \tilde{\mathcal{H}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}} \mid \exists 0 < C < \infty \text{ such that } \|(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]\| < C\}.$$

Corollary C.2 states that the requirement $u_j \in \mathcal{F} = \tilde{\mathcal{H}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1$ can be weakened to $u_j \in \tilde{\mathcal{H}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$ such that the operator $(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]$ is bounded on \mathcal{F} . The set \mathcal{U} in (C.8) is non-empty. We established this in (C.7), showing that $\{u_j \in \tilde{\mathcal{H}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}} \mid \|u_j\|_{\infty} < \infty\} \subset \mathcal{U}$, as $(-\Delta)^{-1}$ is a bounded operator on $\mathcal{H}_{\mathcal{V}}$ [85]. This extension of Theorem C.1 allows for spatially *unbounded flows* with square integrable singularities.

Proof of Corollary C.2. There are three places in the proof of Theorem C.1 which requires a certain amount of regularity in the components u_j of the fluid velocity field \mathbf{u} . One requirement was that the operator $(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]$ be bounded on \mathcal{F} so that A is a maximal (skew-symmetric) normal operator on \mathcal{F} . Another regularity requirement of u_j appeared in the calculation in equation (C.5). The functional $\langle u_j \chi_k \rangle$ in equation (C.5) is well defined for $u_j, \chi_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$, as the Cauchy-Schwartz inequality yields $|\langle u_j \chi_k \rangle| \leq \|u_j\| \|\chi_k\| < \infty$, while the functional $\langle (-\Delta)^{-1} u_j, \chi_k \rangle_1$ in (C.5) is well defined for $u_j \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$ and $\chi_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1$, as $(-\Delta)^{-1} : \mathcal{H}_{\mathcal{V}} \rightarrow \mathcal{H}_{\mathcal{V}}^1$ [12]. However, the intermediate step $\langle u_j \chi_k \rangle = \langle [\Delta \Delta^{-1} u_j] \chi_k \rangle$ required that $\Delta^{-1} u_j$ has square integrable spatial derivatives of order two, i.e., $u_j \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1$. Although, after the integration by parts, this requirement was weakened to $u_j \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$. The final regularity requirement on u_j was in the conditions of the spectral theorem in (A.7). Namely, that $(-\Delta)^{-1} u_j \in \mathcal{F} = \tilde{\mathcal{H}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1$, as well as $(-\Delta)^{-1} u_j \in \mathcal{D}(F)$ and $(-\Delta)^{-1} u_j \in \mathcal{D}(G)$ for $F(\lambda) = (\varepsilon + i\lambda)^{-1}$ and $G(\lambda) = i\lambda(\varepsilon + i\lambda)^{-1}$. However, we demonstrated that $f \in \mathcal{D}(F)$ and $f \in \mathcal{D}(G)$ for all $f \in \mathcal{F}$. Since $(-\Delta)^{-1} : \mathcal{H}_{\mathcal{V}} \rightarrow \mathcal{H}_{\mathcal{V}}^1$ [12], we only require that $u_j \in \tilde{\mathcal{H}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$. This allows for spatially unbounded flows with square integrable singularities. An exposition of the specific details is beyond the scope of the current work. This concludes our proof of Corollary C.2 \square .

C.2. Curl-free vector fields and effective diffusivity. In this section we provide a rigorous mathematical framework for an alternate formulation [6] of the effective parameter problem for advection enhanced diffusion by space-time periodic fluid velocity fields. This approach provides analogous formulas to those displayed in equations (2.11)–(2.14) involving the *curl-free* vector field $\nabla \chi_j$ displayed in equation (2.8) and a maximal (skew-symmetric) normal operator acting on a suitable Hilbert space. Towards this goal, recall the Hilbert spaces $\mathcal{H}_{\mathcal{T}}$ and $\mathcal{H}_{\mathcal{V}}$ given in equation (C.1) and the function space $\tilde{\mathcal{H}}_{\mathcal{T}}$ given in equation (B.3). Now define their d -dimensional analogues over the complex field \mathbb{C} ,

$$(C.9) \quad \mathcal{H}_{\mathcal{T}} = \otimes_{j=1}^d \mathcal{H}_{\mathcal{T}}, \quad \mathcal{H}_{\mathcal{V}} = \otimes_{j=1}^d \mathcal{H}_{\mathcal{V}}, \quad \mathcal{F} = \otimes_{j=1}^d \mathcal{F}.$$

By the Helmholtz theorem [55, 10], the Hilbert space $\mathcal{H}_{\mathcal{V}}$ can be decomposed into mutually orthogonal subspaces of curl-free \mathcal{H}_{\times} , divergence-free \mathcal{H}_{\bullet} , and constant \mathcal{H}_0 vector fields, with $\mathcal{H}_{\mathcal{V}} = \mathcal{H}_{\times} \oplus \mathcal{H}_{\bullet} \oplus \mathcal{H}_0$. The orthogonal projectors associated with this decomposition are given by $\Gamma_{\times} = -\nabla(-\Delta)^{-1}\nabla \cdot$, $\Gamma_{\bullet} = \nabla \times (-\Delta^{-1})\nabla \times$, and $\Gamma_0 = \langle \cdot \rangle$, respectively, satisfying $\mathbf{l} = \Gamma_{\times} + \Gamma_{\bullet} + \Gamma_0$ [28, 64]. Here, $\Delta = \text{diag}(\Delta, \dots, \Delta)$ is the vector Laplacian with inverse $\Delta^{-1} = \text{diag}(\Delta^{-1}, \dots, \Delta^{-1})$, $\langle \cdot \rangle$ denotes space-time averaging over the period cell $\mathcal{T} \times \mathcal{V}$, and \mathbf{l} is the identity operator on $\mathcal{H}_{\mathcal{V}}$. Due to the *curl-free* vector field $\nabla \chi_j$ at the heart of the cell problem in equation (2.8), we will find particular use of the Hilbert space \mathcal{H}_{\times} , which we define as

$$(C.10) \quad \mathcal{H}_{\times} = \{\psi \in \mathcal{H}_{\mathcal{V}} \mid \Gamma \psi = \psi\}, \quad \Gamma = -\nabla(-\Delta)^{-1}\nabla \cdot,$$

where we have denoted Γ_{\times} by Γ for notational simplicity. Analogous to equation (C.3), we define the Hilbert space \mathcal{H} and its everywhere dense subset \mathcal{F} ,

$$(C.11) \quad \mathcal{H} = \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\times}, \quad \mathcal{F} = \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\times}.$$

Denote by $\|\cdot\|$ the norm induced by the the sesquilinear inner-product $\langle \cdot, \cdot \rangle$ associated with the Hilbert space \mathcal{H} , defined by $\langle \psi, \varphi \rangle = \langle \psi \cdot \varphi \rangle$ with $\langle \psi, \varphi \rangle = \langle \varphi, \psi \rangle$. We will henceforth assume that $\mathbf{u}, \nabla \chi_j \in \mathcal{F}$. In the case of a steady fluid velocity field $\mathbf{u}(\mathbf{x})$, we set $\mathcal{H} \equiv \mathcal{F} \equiv \mathcal{H}_{\times}$.

Since the fluid velocity field \mathbf{u} is incompressible, there is a real skew-symmetric matrix $\mathbf{H}(t, \mathbf{x})$ satisfying [4, 5]

$$(C.12) \quad \mathbf{u} = \nabla \cdot \mathbf{H}, \quad \mathbf{H}^T = -\mathbf{H},$$

where \mathbf{H}^T denotes transposition of the matrix \mathbf{H} . Since $\mathbf{u} \in \mathcal{F}$, we have that the components H_{jk} of the matrix \mathbf{H} have square integrable spatial derivatives of order two on the set \mathcal{V} [12]. Due to the skew-symmetry of \mathbf{H} , we have the identity $[\nabla \cdot \mathbf{H}] \cdot \nabla f = \nabla \cdot [\mathbf{H} \nabla f]$. Using this identity and the representation of the velocity field \mathbf{u} in (C.12), the advection-diffusion equation in (2.1) can be written as a diffusion equation [28],

$$(C.13) \quad \partial_t \phi = \nabla \cdot \mathbf{D} \nabla \phi, \quad \phi(0, \mathbf{x}) = \phi_0(\mathbf{x}), \quad \mathbf{D} = \varepsilon \mathbf{I} + \mathbf{H},$$

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

$$(C.14) \quad D_{jk} = \varepsilon \delta_{jk} + H_{jk}, \quad j, k = 1, \dots, d.$$

The cell problem in (2.8) can also be written as the following diffusion equation [28]

$$(C.15) \quad \partial_t \chi_j = \nabla \cdot [\mathbf{D}(\nabla \chi_j + \mathbf{e}_j)], \quad \langle \nabla \chi_k \rangle = 0, \quad \mathbf{D} = \varepsilon \mathbf{I} + \mathbf{H},$$

where $\langle \nabla \chi_k \rangle = 0$ follows from the periodicity of χ_k .

We now recast the first formula in equation (C.15) in a more suggestive, divergence form. Define the operator $\mathbf{T} : \tilde{\mathcal{A}}_{\mathcal{T}} \rightarrow \mathcal{H}_{\mathcal{T}}$ by $(\mathbf{T}\psi)_j = \partial_t \psi_j$, $j = 1, \dots, d$. For $f \in \mathcal{F}$ we have we define

$$(C.16) \quad \nabla(\Delta^{-1})\partial_t f = \Delta^{-1}\mathbf{T}\nabla f,$$

so that [28] $\partial_t \chi_k = \Delta \Delta^{-1} \partial_t \chi_k = \nabla \cdot (\Delta^{-1} \mathbf{T}) \nabla \chi_k$. Define the vector field $\mathbf{E}_k = \nabla \chi_k + \mathbf{e}_k$ and the operator $\boldsymbol{\sigma} = \mathbf{D} - (\Delta^{-1})\mathbf{T} = \varepsilon \mathbf{I} + \mathbf{S}$, where $\mathbf{S} = \mathbf{H} - (\Delta^{-1})\mathbf{T}$ and in the case of a steady fluid velocity field $\mathbf{u}(\mathbf{x})$ we have $\boldsymbol{\sigma} = \mathbf{D}$. With these definitions, equation (C.15) can be written as $\nabla \cdot \boldsymbol{\sigma} \mathbf{E}_k = 0$, $\langle \mathbf{E}_k \rangle = \mathbf{e}_k$, which is equivalent to

$$(C.17) \quad \nabla \cdot \mathbf{J}_k = 0, \quad \nabla \times \mathbf{E}_k = 0, \quad \mathbf{J}_k = \boldsymbol{\sigma} \mathbf{E}_k, \quad \langle \mathbf{E}_k \rangle = \mathbf{e}_k, \quad \boldsymbol{\sigma} = \varepsilon \mathbf{I} + \mathbf{S}.$$

The formulas in (C.17) are precisely the electrostatic version of Maxwell's equations for a conductive medium [37], where \mathbf{E}_k and \mathbf{J}_k are the local electric field and current density, respectively, and $\boldsymbol{\sigma}$ is the local conductivity tensor of the medium. In the analytic continuation method for composites [37], the effective conductivity tensor $\boldsymbol{\sigma}^*$ is defined as

$$(C.18) \quad \langle \mathbf{J}_k \rangle = \boldsymbol{\sigma}^* \langle \mathbf{E}_k \rangle.$$

The linear constitutive relation $\mathbf{J}_k = \boldsymbol{\sigma} \mathbf{e}_k$ in (C.17) relates the local intensity and flux, while that in (D.11) relates the mean intensity and flux. Due to the skew-symmetry of \mathbf{S} , the intensity-flux relationship in (C.17) is similar to that of a Hall medium [45, 28].

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THEOREM C.3. *Let the components D_{jk}^* and σ_{jk}^* , $j, k = 1, \dots, d$, of the effective tensors D^* and σ^* be defined as in equations (C.21)–(C.20) and (C.17)–(D.11), respectively. Then there exists a function space \mathcal{F} on which $\sigma = \varepsilon I + \mathbf{S}$ is a bounded linear operator for all $0 < \varepsilon < \infty$ and, for $\nabla \chi_j \in \mathcal{F}$, D_{jk}^* and σ_{jk}^* are well defined and finite. Moreover, these effective tensors are equivalent up to transposition,*

$$(C.19) \quad \sigma^* = [D^*]^T.$$

In particular, the symmetric part D^ of D^* is equal to that of σ^* and the anti-symmetric part A^* of D^* is equal to the negative of that of σ^* .*

Using this representation of the fluid velocity field, the components S_{jk}^* and A_{jk}^* , $j, k = 1, \dots, d$, of the symmetric S^* and antisymmetric A^* parts of the effective diffusivity tensor D^* can be represented in terms of the \mathcal{H} -inner-product $\langle \cdot, \cdot \rangle$ by the following functional formulas [4, 5]

$$(C.20) \quad S_{jk}^* = \varepsilon(\delta_{jk} + \langle \nabla \chi_j, \nabla \chi_k \rangle), \quad A_{jk}^* = \langle \mathbf{A} \nabla \chi_j, \nabla \chi_k \rangle, \quad \mathbf{A} = \mathbf{\Gamma}[\mathbf{H} - (\Delta^{-1})\mathbf{T}] \mathbf{\Gamma}.$$

Here, $\mathbf{T} = \text{diag}(\partial_t, \dots, \partial_t)$ operates component-wise on d -dimensional vector fields, the inverse of the vector Laplacian Δ is denoted by $\Delta^{-1} = \text{diag}(\Delta^{-1}, \dots, \Delta^{-1})$, where Δ^{-1} is based on convolution with the Green's function for the Laplacian Δ on \mathcal{V} [85].

The formulas in equation (C.20) are obtained by casting the cell problem in (2.8) into a form which parallels the effective parameter problem for transport in composite materials [4, 5]. This allows one to bring to bear well developed mathematical techniques of the analytic continuation method for representing transport in composites [37, 64]. This method provides Stieltjes integral representations for the effective transport coefficients of composite media, involving a spectral measure of a self-adjoint operator which depends only on the composite geometry [37, 67, 64].

Towards this goal, we now transform the cell problem in (2.8) into a divergence equation [28] which immediately yields equation (C.20) and readily leads to a resolvent formula for the curl-free vector field $\nabla \chi_j$, analogous to that for the scalar field χ_j displayed in (2.12). Using the representation of the fluid velocity field given in (C.12), the advection-diffusion equation in (2.1) can be written as a diffusion equation, $\partial_t \phi = \nabla \cdot [\mathbf{D} \nabla \phi]$, where $\mathbf{D}(t, \mathbf{x}) = \varepsilon I + \mathbf{H}(t, \mathbf{x})$ can be viewed as a local diffusivity tensor. The cell problem in (2.8) can also be written as the following diffusion equation [28]

$$(C.21) \quad \partial_t \chi_j = \nabla \cdot [\mathbf{D}(\nabla \chi_j + \mathbf{e}_j)], \quad \langle \nabla \chi_k \rangle = 0, \quad \mathbf{D} = \varepsilon I + \mathbf{H}.$$

Due to the skew-symmetry of the matrix \mathbf{H} , we have the identity $[\nabla \cdot \mathbf{H}] \cdot \nabla \chi_j = \nabla \cdot [\mathbf{H} \nabla \chi_j]$. Now, writing $\partial_t \chi_j = \Delta \Delta^{-1} \partial_t \chi_j = \nabla \cdot (\Delta^{-1} \mathbf{T}) \nabla \chi_j$ and $\mathbf{E}_j = \nabla \chi_j + \mathbf{e}_j$, equation (C.21) can be written in divergence form [28],

$$(C.22) \quad \nabla \cdot [\sigma \mathbf{E}_j] = 0, \quad \langle \mathbf{E}_j \rangle = \mathbf{e}_j, \quad \sigma = \varepsilon I + \mathbf{H} - (\Delta^{-1})\mathbf{T},$$

where we have written $\nabla(\Delta^{-1})\partial_t = \Delta^{-1}\mathbf{T}\nabla$. In terms of the curl-free vector field $\nabla \chi_j$, equation (C.22) is given by $\nabla \cdot [\sigma \nabla \chi_j] = -u_j$. Equation (C.20) now follows from the formula $D_{jk}^* = \varepsilon \delta_{jk} + \langle u_j \chi_k \rangle$ in equation (2.9), yielding

$$(C.23) \quad \langle u_j \chi_k \rangle = -\langle [\nabla \cdot \sigma \nabla \chi_j] \chi_k \rangle = \langle \sigma \nabla \chi_j \cdot \nabla \chi_k \rangle = \varepsilon \langle \nabla \chi_j \cdot \nabla \chi_k \rangle + \langle \mathbf{\Gamma}[\mathbf{H} - (\Delta^{-1})\mathbf{T}] \mathbf{\Gamma} \nabla \chi_j \cdot \nabla \chi_k \rangle,$$

where we have used the periodicity of χ_k and \mathbf{H} in the second equality and the final equality follows from the property $\mathbf{\Gamma} \nabla \chi_j = \nabla \chi_j$ of the *self-adjoint* operator $\mathbf{\Gamma}$ on \mathcal{H} , defined in (C.10).

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Since the function spaces \mathcal{F} and \mathcal{F} differ only in the characterization of the spatial variable \mathbf{x} , we now discuss the relationship between the Hilbert spaces \mathcal{H}_\times and $\mathcal{H}_\mathcal{V}^1$ defined in equations (C.10) and (C.2), respectively, with inner-product induced norms $\|\cdot\|$ and $\|\cdot\|_1$. For $f \in \mathcal{H}_\mathcal{V}^1 \subset L^2(\mathcal{V})$ we have $\Delta^{-1} \Delta f = f$ [85], which implies that $\mathbf{\Gamma} \nabla f = \nabla f$ and $\|\nabla f\|^2 = \langle \nabla f \cdot \nabla f \rangle = \|f\|_1^2 < \infty$. Consequently, for every $f \in \mathcal{H}_\mathcal{V}^1$ we have $\nabla f \in \mathcal{H}_\times$. Conversely, $\psi \in \mathcal{H}_\times$ implies that $\psi = \mathbf{\Gamma} \psi = \nabla f$, where we have defined the scalar-valued function $f = \Delta^{-1} \nabla \cdot \psi$. Since $\psi = \nabla f$, the $\mathcal{H}_\mathcal{V}^1$ norm of f satisfies $\|f\|_1^2 = \langle \psi \cdot \psi \rangle = \|\psi\|^2 < \infty$ so that $f \in \mathcal{H}_\mathcal{V}^1$. Moreover, f is uniquely determined by ψ up to equivalence class, since if $f_1 = \Delta^{-1} \nabla \cdot \psi$ and $f_2 = \Delta^{-1} \nabla \cdot \psi$ then $\mathbf{\Gamma} \psi = \psi$ implies that $\|f_1 - f_2\|_1 = \|\psi - \psi\| = 0$. Consequently, for every $\psi \in \mathcal{H}_\times$ there exists unique $f \in \mathcal{H}_\mathcal{V}^1$ such that $\psi = \nabla f$. In summary, the Hilbert spaces $\mathcal{H}_\mathcal{V}^1$ and \mathcal{H}_\times are in one-to-one isometric correspondence, which we denote by $\mathcal{H}_\mathcal{V}^1 \sim \mathcal{H}_\times$. This, in turn, implies that $\mathcal{F} \sim \mathcal{F}$. IS $\tilde{\mathcal{A}}_T \sim \tilde{\mathcal{A}}_T$?

We are primarily concerned with fluid velocity fields \mathbf{u} such that $0 < D_{kk}^* < \infty$ for all $0 < \varepsilon < \infty$. Consequently, in view of equation (C.20), we require that the (weakly) curl-free vector field $\nabla \chi_k$ satisfies $\nabla \chi_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\times} \subset \mathcal{H}_{\mathcal{TV}}$, so that it is bounded in the norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{TV}}$ -inner-product [33], $\|\nabla \chi_k\| < \infty$. Defining the (weakly) divergence-free vector field $\mathbf{J}_k = \boldsymbol{\sigma} \mathbf{e}_k$ in (C.17) as a member of a subset of $\mathcal{H}_{\mathcal{TV}}$ is technically difficult, due to the *unboundedness* of the linear operator $\boldsymbol{\sigma} = \mathbf{D} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ on this space. We now explore the properties of this operator in more detail.

Since \mathcal{V} is a bounded domain, $(\boldsymbol{\Delta}^{-1})$ is a compact operator [85] on the Hilbert space $L^2(\mathcal{V})$. Hence $(\boldsymbol{\Delta}^{-1})$ is a compact operator on the Hilbert space $\mathcal{H}_{\mathcal{V}}$, and is consequently bounded in the operator norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{TV}}$ -inner-product [79, 87, 85], when considered as an operator on $\mathcal{H}_{\mathcal{TV}}$. We have already assumed for the convergence $\phi^\delta \rightarrow \bar{\phi}$, as $\delta \rightarrow 0$, that the flow matrix $\mathbf{H}(t, \mathbf{x})$ is periodic on $\mathcal{T} \times \mathcal{V}$. We will also assume that it is (component-wise) mean-zero and bounded in operator norm, and that its component-wise time derivative \mathbf{TH} is also bounded on $\mathcal{H}_{\mathcal{TV}}$

$$(C.24) \quad \langle \mathbf{H} \rangle = 0, \quad \|\mathbf{H}\| < \infty, \quad \|\mathbf{TH}\| < \infty.$$

This implies that $\mathbf{D} = \varepsilon \mathbf{I} + \mathbf{H}$ is also bounded for all $0 < \varepsilon < \infty$. Consequently, in the case of a time-independent velocity field \mathbf{u} , where $\boldsymbol{\sigma} = \mathbf{D}$, the linear operator $\boldsymbol{\sigma}$ is bounded. This and $\|\nabla \chi_k\| < \infty$ implies that $\mathbf{J}_k \in \mathcal{H}_{\bullet}$. Therefore, in the case of a time-dependent velocity field, under the assumptions of (E.3), the unboundedness of $\boldsymbol{\sigma} = \mathbf{D} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ on $\mathcal{H}_{\mathcal{TV}}$ is due to the unboundedness of \mathbf{T} on $\mathcal{H}_{\mathcal{T}}$.

, which provides the existence of the promised integral representation for \mathbf{D}^* , involving a spectral measure associated with Φ . It is therefore necessary that we find a domain $D(\Phi)$ on which Φ is self-adjoint.

Appendix D. Curl-Free Fields. For d -dimensional, mean-zero, incompressible flows \mathbf{u} , there is a real (non-dimensional) skew-symmetric matrix $\mathbf{H}(t, \mathbf{x})$ such that

$$(D.1) \quad \mathbf{u} = \nabla \cdot \mathbf{H}, \quad \mathbf{H}^T = -\mathbf{H},$$

where \mathbf{H}^T denotes transposition of the matrix \mathbf{H} . Using this representation of the velocity field \mathbf{u} , equation (2.1) can be written as a diffusion equation,

$$(D.2) \quad \partial_t \phi = \nabla \cdot \mathbf{D} \nabla \phi, \quad \phi(0, \mathbf{x}) = \phi_0(\mathbf{x}), \quad \mathbf{D} = \varepsilon \mathbf{I} + \mathbf{H},$$

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

$$(D.3) \quad \varepsilon_{jk} = \varepsilon \delta_{jk} + \mathbf{H}_{jk}, \quad j, k = 1, \dots, d.$$

We denote by \mathbf{I} the identity operator on all linear spaces in question.

We are interested in the dynamics of ϕ in (C.13) for *large* length and time scales, and when the initial density ϕ_0 is slowly varying relative to the velocity field \mathbf{u} . Anticipating that ϕ will have diffusive dynamics, we re-scale space and time by $\mathbf{x} \rightarrow \mathbf{x}/\delta$ and $t \rightarrow t/\delta^2$, respectively. For periodic diffusivity coefficients in (C.13) which are uniformly elliptic but not necessarily symmetric, it can be shown [28] that, as $\delta \rightarrow 0$, the associated solution $\phi^\delta(t, \mathbf{x})$ of (C.13) converges to $\bar{\phi}(t, \mathbf{x})$, which satisfies the following diffusion equation involving a (constant) effective diffusivity tensor \mathbf{D}^*

$$(D.4) \quad \partial_t \bar{\phi} = \nabla \cdot \mathbf{D}^* \nabla \bar{\phi}, \quad \bar{\phi}(0, \mathbf{x}) = \phi_0(\mathbf{x}).$$

The components $D_{jk}^* = \mathbf{D}^* \mathbf{e}_j \cdot \mathbf{e}_k$ of the effective tensor \mathbf{D}^* are given by $D_{jk}^* = \varepsilon \delta_{jk} + \langle u_j \chi_k \rangle$. For each standard basis vector \mathbf{e}_k , $k = 1, \dots, d$, the function $\chi_k = \chi_k(t, \mathbf{x}; \mathbf{e}_k)$ satisfies [28] the cell problem

$$(D.5) \quad \partial_t \chi_k = \nabla \cdot \mathbf{D}(\nabla \chi_k + \mathbf{e}_k), \quad \langle \nabla \chi_k \rangle = 0.$$

The symmetric \mathbf{D}^* and anti-symmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* are defined by

$$(D.6) \quad \mathbf{D}^* = \mathbf{S}^* + \mathbf{A}^*, \quad \mathbf{S}^* = \frac{1}{2} (\mathbf{D}^* + [\mathbf{D}^*]^T), \quad \mathbf{A}^* = \frac{1}{2} (\mathbf{D}^* - [\mathbf{D}^*]^T).$$

The components S_{jk}^* and A_{jk}^* , $j, k = 1, \dots, d$, of \mathbf{D}^* and \mathbf{A}^* can be written in terms of the following functionals involving the *real-valued* vector field $\nabla \chi_k$

$$(D.7) \quad S_{jk}^* = \varepsilon(\delta_{jk} + \langle \nabla \chi_j \cdot \nabla \chi_k \rangle), \quad A_{jk}^* = \langle \mathbf{S} \nabla \chi_j \cdot \nabla \chi_k \rangle, \quad \mathbf{S} = \mathbf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}, \quad \mathbf{T} = \partial_t \mathbf{I},$$

where $\psi \cdot \varphi = \psi^\dagger \varphi$ denotes the $\ell^2(\mathbb{C}^N)$ inner-product and \dagger is the operation of complex-conjugate-transpose. Here, $\mathbf{T} = \text{diag}(\partial_t, \dots, \partial_t)$ operates component-wise on vector fields, $\Delta^{-1} = \text{diag}(\Delta^{-1}, \dots, \Delta^{-1})$ is the inverse of the vector Laplacian, and the inverse operation Δ^{-1} is based on convolution with the Green's function for the Laplacian Δ on \mathcal{V} [85]. We stress that, while the effective diffusivity tensor \mathbf{D}^* is not symmetric in general, only its symmetric part appears in the homogenized equation [60] in (2.3).

Due to the fact that the vector field $\nabla \chi_j$ is *real-valued*, we have that $\langle \nabla \chi_j \cdot \nabla \chi_k \rangle = \langle \nabla \chi_k \cdot \nabla \chi_j \rangle$. From equation (C.20) this clearly implies that the tensor \mathbf{D}^* is symmetric, $\mathbf{S}_{jk}^* = \mathbf{S}_{kj}^*$. Moreover, equation (C.20) demonstrates that the effective transport of the tracer ϕ in the principle directions \mathbf{e}_k , $k = 1, \dots, d$, is always *enhanced* by the presence of an incompressible velocity field, $\mathbf{D}_{kk}^* = \mathbf{S}_{kk}^* \geq \varepsilon$. The equality $\mathbf{D}_{kk}^* = \mathbf{S}_{kk}^*$ follows from the skew-symmetry of \mathbf{A}^* , so that $\mathbf{A}_{kj}^* = -\mathbf{A}_{jk}^*$ and $\mathbf{A}_{kk}^* = 0$. This, in turn, follows from the skew-symmetry of the operator \mathbf{S} (see Section F.4), $\mathbf{A}_{jk}^* = \langle \mathbf{S} \nabla \chi_j \cdot \nabla \chi_k \rangle = -\langle \mathbf{S} \nabla \chi_k \cdot \nabla \chi_j \rangle = -\mathbf{A}_{kj}^*$ and

$$(D.8) \quad \mathbf{A}_{kk}^* = \langle \mathbf{S} \nabla \chi_k \cdot \nabla \chi_k \rangle = -\langle \mathbf{S} \nabla \chi_k \cdot \nabla \chi_k \rangle = 0.$$

In Section E we discuss the properties of the linear operator \mathbf{S} and the vector field $\nabla \chi_j$ in more detail.

We now recast equations (C.21) and (C.20) into a form which parallels the effective parameter problem for transport in composites. This allows us to bring to bear on the effective parameter problem for advective diffusion, the well developed mathematical techniques of the analytic continuation method for characterizing effective transport in composite media [37, 64]. This method gives a Hilbert space formulation of the effective parameter problem and provides an integral representation for the effective transport coefficients of composites, involving a *spectral measure* of a self-adjoint operator which depends only on the composite geometry [37, 67, 64]. Here we establish a correspondence between this effective parameter problem and that for enhanced diffusive transport by advective velocity fields. In Section E, we formulate the Hilbert space framework associated with advective diffusion, and employ it to obtain a resolvent representation of the vector field $\nabla \chi_k$ in (C.21). In Section F we utilize this mathematical framework to obtain integral representations for \mathbf{D}^* and \mathbf{A}^* , involving a spectral measure which depends only on the fluid velocity field \mathbf{u} .

Toward this goal, we recast the first formula in equation (C.21) in a more suggestive, divergence form. Using the notation from equation (C.20) we write

$$(D.9) \quad \nabla(\Delta^{-1})\partial_t = \Delta^{-1}\mathbf{T}\nabla,$$

so that [28] $\partial_t \chi_k = \Delta \Delta^{-1} \partial_t \chi_k = \nabla \cdot (\Delta^{-1} \mathbf{T}) \nabla \chi_k$. Define the vector field $\mathbf{e}_k = \nabla \chi_k + \mathbf{e}_k$ and the operator $\boldsymbol{\sigma} = \mathbf{D} - (\Delta^{-1})\mathbf{T} = \varepsilon \mathbf{I} + \mathbf{S}$, where $\boldsymbol{\sigma} = \mathbf{D} = \varepsilon \mathbf{I} + \mathbf{H}$ in the case of steady fluid velocity fields. With these definitions, equation (C.21) may be written as $\nabla \cdot \boldsymbol{\sigma} \mathbf{e}_k = 0$, $\langle \mathbf{e}_k \rangle = \mathbf{e}_k$, which is equivalent to

$$(D.10) \quad \nabla \cdot \mathbf{J}_k = 0, \quad \nabla \times \mathbf{e}_k = 0, \quad \mathbf{J}_k = \boldsymbol{\sigma} \mathbf{e}_k, \quad \langle \mathbf{e}_k \rangle = \mathbf{e}_k, \quad \boldsymbol{\sigma} = \varepsilon \mathbf{I} + \mathbf{S}.$$

The formulas in (C.17) are precisely the electrostatic version of Maxwell's equations for a conductive medium [37], where \mathbf{e}_k and \mathbf{J}_k are the local electric field and current density, respectively, and $\boldsymbol{\sigma}$ is the local conductivity tensor of the medium. In the analytic continuation method for composites, the effective conductivity tensor $\boldsymbol{\sigma}^*$ is defined as

$$(D.11) \quad \langle \mathbf{J}_k \rangle = \boldsymbol{\sigma}^* \langle \mathbf{e}_k \rangle.$$

The linear constitutive relation $\mathbf{J}_k = \boldsymbol{\sigma} \mathbf{e}_k$ in (C.17) relates the local intensity and flux, while that in (D.11) relates the mean intensity and flux. Due to the skew-symmetry of \mathbf{S} , the intensity-flux relationship in (C.17) is similar to that of a Hall medium [45].

For the (constant) tensors \mathbf{D}^* and $\boldsymbol{\sigma}^*$ to be meaningful, the averages which define these effective quantities in (C.20) and (D.11) must be well defined and finite. For example, in order for the diagonal components \mathbf{D}_{kk}^* , $k = 1, \dots, d$, of \mathbf{D}^* to be well defined and finite, the vector field $\nabla \chi_k$ must be Lebesgue measurable and square integrable on $\mathcal{T} \times \mathcal{V}$. Moreover, for the components \mathbf{A}_{jk}^* , $j \neq k = 1, \dots, d$, of \mathbf{A}^* to be well defined and finite, we must also have that the operator \mathbf{S} is bounded in some sense so that $\mathbf{S} \nabla \chi_j \cdot \nabla \chi_k$ is Lebesgue integrable on $\mathcal{T} \times \mathcal{V}$. In other words, we must define the vector field $\nabla \chi_j$ as a member of a suitable space of functions so that the components of the tensors \mathbf{D}^* and $\boldsymbol{\sigma}^*$ are well defined and have finite values. In Section E we discuss these important details at length and prove the following theorem.

THEOREM D.1. *Let the components D_{jk}^* and σ_{jk}^* , $j, k = 1, \dots, d$, of the effective tensors D^* and σ^* be defined as in equations (C.21)–(C.20) and (C.17)–(D.11), respectively. Then there exists a function space \mathcal{F} on which $\sigma = \varepsilon I + \mathbf{S}$ is a bounded linear operator for all $0 < \varepsilon < \infty$ and, for $\nabla\chi_j \in \mathcal{F}$, D_{jk}^* and σ_{jk}^* are well defined and finite. Moreover, these effective tensors are equivalent up to transposition,*

$$(D.12) \quad \sigma^* = [D^*]^T.$$

In particular, the symmetric part D^ of D^* is equal to that of σ^* and the anti-symmetric part A^* of D^* is equal to the negative of that of σ^* .*

Theorem C.3 places the effective parameter problems for transport in composites and that for transport by advective diffusion on common mathematical footing, for both cases of time-independent and time-dependent velocity fields \mathbf{u} . The validity of Theorem C.3 follows by adapting the Hilbert space formulation of the analytic continuation method to treat the effective transport properties of advective diffusion, which is the topic of Section E. This Hilbert space formulation of the effective parameter problem also leads to integral representations for D^* and A^* , which is the topic of Section F.

Appendix E. Hilbert space and resolvent representation. In this section we explore the mathematical properties of the skew-symmetric operator \mathbf{S} introduced in equation (C.20) and construct a function space \mathcal{F} such that for $\nabla\chi_k \in \mathcal{F}$ equation (C.19) holds and is well defined. We do so by providing an abstract Hilbert space formulation of the effective parameter problem for advective diffusion. We utilize this mathematical framework and equation (C.21) to obtain a resolvent representation of the vector field $\nabla\chi_k$, involving an anti-symmetric operator \mathbf{A} which is closely related to \mathbf{S} , where we use the terms skew-symmetric and anti-symmetric interchangeably. Using the results of this section, we derive in Section F integral representations for the symmetric D^* and anti-symmetric A^* parts of the effective diffusivity tensor D^* , involving a *spectral measure* associated with \mathbf{A} .

Consider the Hilbert spaces over the complex field \mathbb{C} $L_d^2(\mathcal{T}) = \otimes_{n=1}^d L^2(\mathcal{T})$ and $L_d^2(\mathcal{V}) = \otimes_{n=1}^d L^2(\mathcal{V})$ of Lebesgue measurable, square integrable, vector-valued functions [33], where $\mathcal{T} \subset \mathbb{R}$ and $\mathcal{V} \subset \mathbb{R}^d$. Now consider the associated Hilbert spaces $\mathcal{H}_{\mathcal{T}} \subset L_d^2(\mathcal{T})$ and $\mathcal{H}_{\mathcal{V}} \subset L_d^2(\mathcal{V})$ of periodic vector-valued functions with temporal periodicity T on the interval $\mathcal{T} = (0, T)$ and spatial periodicities V_j , $j = 1, \dots, d$, on the d -dimensional region $\mathcal{V} = (0, V_1) \times \dots \times (0, V_d)$, respectively, as well as their direct product $\mathcal{H}_{\mathcal{TV}}$,

$$(E.1) \quad \mathcal{H}_{\mathcal{TV}} = \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}, \quad \mathcal{H}_{\mathcal{T}} = \{\psi \in L_d^2(\mathcal{T}) \mid \psi(0) = \psi(T)\}, \quad \mathcal{H}_{\mathcal{V}} = \{\psi \in L_d^2(\mathcal{V}) \mid \psi(0) = \psi(\mathbf{u})\},$$

where we have defined $\mathbf{u} = (V_1, \dots, V_d)$. Denote by $\langle \cdot, \cdot \rangle$ the sesquilinear inner-product associated with the Hilbert space $\mathcal{H}_{\mathcal{TV}}$, which is defined by $\langle \psi, \varphi \rangle = \langle \bar{\psi} \cdot \varphi \rangle$ with $\langle \bar{\psi}, \varphi \rangle = \overline{\langle \varphi, \bar{\psi} \rangle}$, where \bar{a} denotes complex conjugation for $a \in \mathbb{C}$ and $(\bar{\psi})_j = \overline{\psi_j}$, $j = 1, \dots, d$. By the Helmholtz theorem [55, 10], the Hilbert space $\mathcal{H}_{\mathcal{V}}$ in (C.9) can be decomposed into mutually orthogonal subspaces of curl-free \mathcal{H}_{\times} , divergence-free \mathcal{H}_{\bullet} , and constant \mathcal{H}_0 vector fields, with associated orthogonal projectors Γ_{\times} , Γ_{\bullet} , and Γ_0 , respectively, [28, 64]

$$(E.2) \quad \begin{aligned} \mathcal{H}_{\mathcal{V}} &= \mathcal{H}_{\times} \oplus \mathcal{H}_{\bullet} \oplus \mathcal{H}_0, \quad \mathbf{I} = \Gamma_{\times} + \Gamma_{\bullet} + \Gamma_0, \\ \Gamma_{\times} &= \nabla(\Delta^{-1})\nabla \cdot, \quad \Gamma_{\bullet} = -\nabla \times (\Delta^{-1})\nabla \times, \quad \Gamma_0 = \langle \cdot \rangle, \\ \mathcal{H}_{\times} &= \{\psi \mid \nabla \times \psi = 0 \text{ weakly}\}, \quad \mathcal{H}_{\bullet} = \{\psi \mid \nabla \cdot \psi = 0 \text{ weakly}\}, \quad \mathcal{H}_0 = \{\psi \mid \psi = \langle \psi \rangle\}. \end{aligned}$$

We are primarily concerned with fluid velocity fields \mathbf{u} such that $0 < D_{kk}^* < \infty$ for all $0 < \varepsilon < \infty$. Consequently, in view of equation (C.20), we require that the (weakly) curl-free vector field $\nabla\chi_k$ satisfies $\nabla\chi_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\times} \subset \mathcal{H}_{\mathcal{TV}}$, so that it is bounded in the norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{TV}}$ -inner-product [33], $\|\nabla\chi_k\| < \infty$. Defining the (weakly) divergence-free vector field $\mathbf{J}_k = \sigma \mathbf{e}_k$ in (C.17) as a member of a subset of $\mathcal{H}_{\mathcal{TV}}$ is technically difficult, due to the *unboundedness* of the linear operator $\sigma = D - (\Delta^{-1})\mathbf{T}$ on this space. We now explore the properties of this operator in more detail.

Since \mathcal{V} is a bounded domain, (Δ^{-1}) is a compact operator [85] on the Hilbert space $L^2(\mathcal{V})$. Hence (Δ^{-1}) is a compact operator on the Hilbert space $\mathcal{H}_{\mathcal{V}}$, and is consequently bounded in the operator norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{TV}}$ -inner-product [79, 87, 85], when considered as an operator on $\mathcal{H}_{\mathcal{TV}}$. We have already assumed for the convergence $\phi^\delta \rightarrow \bar{\phi}$, as $\delta \rightarrow 0$, that the flow matrix $\mathbf{H}(t, \mathbf{x})$ is periodic on $\mathcal{T} \times \mathcal{V}$. We will also assume that it is (component-wise) mean-zero and bounded in operator norm, and that its component-wise time derivative \mathbf{TH} is also bounded on $\mathcal{H}_{\mathcal{TV}}$

$$(E.3) \quad \langle \mathbf{H} \rangle = 0, \quad \|\mathbf{H}\| < \infty, \quad \|\mathbf{TH}\| < \infty.$$

This implies that $D = \varepsilon I + H$ is also bounded for all $0 < \varepsilon < \infty$. Consequently, in the case of a time-independent velocity field \mathbf{u} , where $\sigma = D$, the linear operator σ is bounded. This and $\|\nabla\chi_k\| < \infty$ implies that $\mathbf{J}_k \in \mathcal{H}_\bullet$. Therefore, in the case of a time-dependent velocity field, under the assumptions of (E.3), the unboundedness of $\sigma = D - (\Delta^{-1})\mathbf{T}$ on $\mathcal{H}_{\mathcal{T}\mathcal{V}}$ is due to the unboundedness of \mathbf{T} on $\mathcal{H}_{\mathcal{T}}$.

Proof of Theorem C.3. As a linear operator acting on the function space $\mathcal{F}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$, by construction, $\sigma = D - (\Delta^{-1})\mathbf{T}$ is bounded in operator norm. Recall from (C.17) that $\mathbf{J}_k = \sigma \mathbf{e}_k$ with $\mathbf{e}_k = \nabla\chi_k + \mathbf{e}_k$. It is clear that $\sigma \mathbf{e}_k = D\mathbf{e}_k$, and is bounded by equation (E.3). Consequently, if $\nabla\chi_k \in \mathcal{F}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$ then \mathbf{J}_k is Lebesgue measurable and also bounded in norm on $\mathcal{H}_{\mathcal{T}\mathcal{V}}$. We have already established that $\nabla\chi_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_\times$. Therefore, this and equation (C.21) suggest that we consider the curl-free, mean-zero vector field $\nabla\chi_k$ as a member of the function space $\mathcal{F} \subset \mathcal{F}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$,

$$(E.4) \quad \mathcal{F} = \{\psi \in \mathcal{F}_{\mathcal{T}} \otimes \mathcal{H}_\times \mid \langle \psi \rangle = 0\},$$

which will be used extensively. We stress that \mathcal{F} is *not* a Hilbert space, and is instead a dense subset of the Hilbert space $\mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_\times$. We will henceforth assume that $\nabla\chi_k \in \mathcal{F}$. In the case of a time-independent velocity field \mathbf{u} we set $\mathcal{F}_{\mathcal{T}} = \emptyset$ in (E.4), so that $\psi \in \mathcal{F}$ implies $\psi \in \mathcal{H}_\times$ with $\langle \psi \rangle = 0$. To summarize, since σ is bounded on \mathcal{F} and $\nabla\chi_k \in \mathcal{F}$, we have that the divergence-free vector field $\mathbf{J}_k = \sigma \mathbf{e}_k$ is also bounded $\|\mathbf{J}_k\| < \infty$, thus $\mathbf{J}_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_\bullet$.

By the mutual orthogonality of the Hilbert spaces \mathcal{H}_\times and \mathcal{H}_\bullet in equation (C.10), $\nabla\chi_k \in \mathcal{F}$, $\mathbf{J}_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_\bullet$, and Fubini's theorem [33] imply that $\langle \mathbf{J}_j \cdot \nabla\chi_k \rangle = 0$ for every $j, k = 1, \dots, d$. This is trivially satisfied in the case of a time-independent velocity field \mathbf{u} , since in this case $\sigma = D$ is bounded so that $\mathbf{J}_j \in \mathcal{H}_\bullet$ for $\nabla\chi_k \in \mathcal{F}$. In either case, as $\mathbf{e}_k = \nabla\chi_k + \mathbf{e}_k$, we have $\langle \mathbf{J}_j \cdot \mathbf{e}_k \rangle = \langle \mathbf{J}_j \cdot \mathbf{e}_k \rangle$. Equations (C.17) and (D.11) then imply that the components $\sigma_{jk}^* = \sigma^* \mathbf{e}_j \cdot \mathbf{e}_k = \langle \sigma \mathbf{e}_j \cdot \mathbf{e}_k \rangle$ of the effective tensor σ^* can be expressed as $\sigma_{jk}^* = \langle \sigma \mathbf{e}_j \cdot \mathbf{e}_k \rangle$, with $\sigma = \varepsilon I + \mathbf{S}$ and $\mathbf{S} = H - (\Delta^{-1})\mathbf{T}$. Consequently,

$$(E.5) \quad \sigma_{jk}^* = \varepsilon \langle \mathbf{e}_j \cdot \mathbf{e}_k \rangle + \langle \mathbf{S} \mathbf{e}_j \cdot \mathbf{e}_k \rangle.$$

The property $\langle \nabla\chi_k \rangle = 0$ in (C.21), and equation (C.20) together imply that

$$(E.6) \quad \varepsilon \langle \mathbf{e}_j \cdot \mathbf{e}_k \rangle = \varepsilon [\langle \nabla\chi_j \cdot \nabla\chi_k \rangle + \langle \nabla\chi_j \cdot \mathbf{e}_k \rangle + \langle \mathbf{e}_j \cdot \nabla\chi_k \rangle + \langle \mathbf{e}_j \cdot \mathbf{e}_k \rangle] = \varepsilon (\langle \nabla\chi_j \cdot \nabla\chi_k \rangle + \delta_{jk}) = S_{jk}^*.$$

From the definition of $\mathbf{S} = H - (\Delta^{-1})\mathbf{T}$ in equation (C.20) we have that $\mathbf{S} \mathbf{e}_j = H \mathbf{e}_j$. Consequently, $\langle \mathbf{S} \mathbf{e}_j \cdot \mathbf{e}_k \rangle = \langle H \mathbf{e}_j \cdot \mathbf{e}_k \rangle = 0$, since by equation (E.3) the matrix H is (component-wise) mean-zero. Also, by the definition $\mathbf{u} = \nabla \cdot H$ in (C.12) and the periodicity of H and χ_k , we also have $\langle H \mathbf{e}_j \cdot \nabla\chi_k \rangle = -\langle u_j \chi_k \rangle$ via integration by parts. Therefore, by the skew-symmetry of \mathbf{S} on \mathcal{F} , the symmetries $S_{kj}^* = S_{jk}^*$ and $A_{kj}^* = -A_{jk}^*$, and equations (C.20), (F.24), and (C.23), we have

$$(E.7) \quad \begin{aligned} \langle \mathbf{S} \mathbf{e}_j \cdot \mathbf{e}_k \rangle &= \langle \mathbf{S} \nabla\chi_j \cdot \nabla\chi_k \rangle + \langle \mathbf{S} \nabla\chi_j \cdot \mathbf{e}_k \rangle + \langle \mathbf{S} \mathbf{e}_j \cdot \nabla\chi_k \rangle + \langle \mathbf{S} \mathbf{e}_j \cdot \mathbf{e}_k \rangle \\ &= A_{jk}^* - \langle \nabla\chi_j \cdot H \mathbf{e}_k \rangle + \langle H \mathbf{e}_j \cdot \nabla\chi_k \rangle \\ &= A_{jk}^* + \langle \chi_j u_k \rangle - \langle u_j \chi_k \rangle \\ &= A_{jk}^* + [A_{kj}^* + S_{kj}^* - \varepsilon \delta_{kj}] - [A_{jk}^* + S_{jk}^* - \varepsilon \delta_{jk}] \\ &= -A_{jk}^*. \end{aligned}$$

In summary, from equations (E.5)–(E.7) and the symmetries $S_{jk}^* = S_{kj}^*$ and $A_{kj}^* = -A_{jk}^*$ we have that

$$(E.8) \quad \sigma_{jk}^* = S_{jk}^* - A_{jk}^* = S_{kj}^* + A_{kj}^* = D_{kj}^*,$$

which is equivalent to equation (C.19). This concludes our proof of Theorem C.3 \square .

We conclude this section with a derivation of the following resolvent formula for $\nabla\chi_k$, involving the orthogonal projection operator $\Gamma_\times = \nabla(\Delta^{-1})\nabla \cdot$ onto curl-free fields in (C.10),

$$(E.9) \quad \nabla\chi_j = (\varepsilon I + \mathbf{A})^{-1} \mathbf{g}_j = (\varepsilon I + \imath \mathbf{M})^{-1} \mathbf{g}_j, \quad \mathbf{A} = \Gamma \mathbf{S} \Gamma, \quad \mathbf{M} = -\imath \mathbf{A}, \quad \mathbf{g}_j = -\Gamma H \mathbf{e}_j,$$

where $\iota = \sqrt{-1}$ and we have defined $\mathbf{\Gamma} = \mathbf{\Gamma}_\times$ for notational simplicity. Equation (E.9) follows from applying the integro-differential operator $\nabla(\Delta^{-1})$ to $\nabla \cdot \boldsymbol{\sigma} \mathbf{e}_j = 0$ in equation (C.17), with $\mathbf{e}_j = \nabla \chi_j + \mathbf{e}_j$ and $\boldsymbol{\sigma} = \varepsilon \mathbf{I} + \mathbf{S}$, yielding

$$(E.10) \quad \mathbf{\Gamma}(\varepsilon \mathbf{I} + \mathbf{S})\nabla \chi_j = -\mathbf{\Gamma} \mathbf{H} \mathbf{e}_j,$$

since $\mathbf{\Gamma} \mathbf{e}_j = 0$ and $\mathbf{S} \mathbf{e}_j = \mathbf{H} \mathbf{e}_j$. The equivalence of equations (E.9) and (E.10) can be seen by noting that $\nabla \chi_j \in \mathcal{F}$ implies $\mathbf{\Gamma} \nabla \chi_j = \nabla \chi_j$. We stress that the property $\mathbf{\Gamma} \nabla \chi_j = \nabla \chi_j$ implies that $\mathbf{A} \nabla \chi_j = \mathbf{\Gamma} \mathbf{S} \mathbf{\Gamma} \nabla \chi_j = \mathbf{\Gamma} \mathbf{S} \nabla \chi_j = (\mathbf{\Gamma} \mathbf{H} - \Delta^{-1} \mathbf{T}) \nabla \chi_j$.

It is worth mentioning that taking the $\ell^2(\mathbb{C}^N)$ inner-product of both sides of equation (E.10) with $\nabla \chi_k$, averaging, using the properties $\mathbf{\Gamma} \nabla \chi_j = \nabla \chi_j$ and $\langle \mathbf{\Gamma} \boldsymbol{\psi} \cdot \boldsymbol{\varphi} \rangle = \langle \boldsymbol{\psi} \cdot \mathbf{\Gamma} \boldsymbol{\varphi} \rangle$ for $\boldsymbol{\psi}, \boldsymbol{\varphi} \in \mathcal{H}_V$, and integrating by parts, yields equation (C.23). Moreover, the condition $\langle \mathbf{J}_j \cdot \nabla \chi_k \rangle = 0$ is also equivalent to equation (C.23).

In Section F.4 we show that \mathbf{A} in (E.9) acts as an anti-symmetric linear operator on the Hilbert space \mathcal{H}_{TV} , $\langle \mathbf{A} \boldsymbol{\psi} \cdot \boldsymbol{\varphi} \rangle = \langle \boldsymbol{\psi} \cdot \mathbf{A}^* \boldsymbol{\varphi} \rangle = -\langle \boldsymbol{\psi} \cdot \mathbf{A} \boldsymbol{\varphi} \rangle$. Therefore, \mathbf{A} commutes with its (Hilbert space) adjoint $\mathbf{A}^* = -\mathbf{A}$ (not to be confused with an effective tensor) and is therefore an example of a *normal* operator [87]. Consequently, due to the sesquilinearity of the \mathcal{H}_{TV} -inner-product, $\mathbf{M} = -\iota \mathbf{A}$ acts as a *symmetric* operator, $\mathbf{M}^* = \mathbf{M}$ [79, 87]. Moreover, on the function space \mathcal{F} , \mathbf{A} is a *maximal* normal operator and \mathbf{M} is *self-adjoint* [87]. In Section F we examine these properties of \mathbf{A} and \mathbf{M} in more detail and demonstrate how equation (E.9) and the spectral theory of such operators lead to integral representations for the symmetric \mathbf{D}^* and anti-symmetric \mathbf{A}^* parts of \mathbf{D}^* .

Appendix F. Integral representations of the effective diffusivity. In this section, we employ the Hilbert space formulation of the effective parameter problem discussed in Section E above, to provide integral representations for the symmetric \mathbf{D}^* and anti-symmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* , for steady and dynamic flows. In the general (infinite dimensional) setting, these integral representations involve a *spectral measure* $d\boldsymbol{\mu}$ associated with the (maximal) normal operator $\mathbf{A} = \mathbf{\Gamma} \mathbf{S} \mathbf{\Gamma}$ on \mathcal{F} , or equivalently the self-adjoint operator $\mathbf{M} = -\iota \mathbf{A}$, and follow from the spectral theorem for such linear operators [79, 87] and the resolvent formula for $\nabla \chi_k$ given in equation (E.9). The derivation of these integral representations for \mathbf{D}^* and \mathbf{A}^* is the topic of Section F.1. In Section ?? we discuss an important alternate formulation of the effective parameter problem, where the spatial Hilbert space \mathcal{H}_\times is replaced by a Sobolev space \mathcal{H}_V^1 . In Section F.2 we demonstrate that the two approaches are equivalent, and are in isometric correspondence. The spectral measures underlying these integral representations have discrete and continuous components. In Section F.7 we review this theory and provide an explicit derivation of the discrete component of these integrals, by eigenfunction expansion. In Sections ?? and ?? we discuss the mathematical framework of these two approaches in the finite dimensional setting, where the underlying operators are given by matrices. This spectral analysis illuminates a great deal of structure regarding the spectral measure $d\boldsymbol{\mu}$ in this matrix setting. This structure is utilized in Section 5 to formulate an efficient and stable numerical algorithm for the explicit computation of \mathbf{D}^* and \mathbf{A}^* for model velocity fields \mathbf{u} , by the direct computation of $d\boldsymbol{\mu}$ in terms of the eigenvalues and eigenvectors of \mathbf{A} .

F.1. General infinite dimensional setting - curl free. In the general Hilbert space setting, there are significant differences in the theory between the case of steady flows, where $\mathbf{S} = \mathbf{H}$ is *bounded* on the Hilbert space \mathcal{H}_V , and the case of dynamic flows, where $\mathbf{S} = \mathbf{H} - (\Delta^{-1}) \mathbf{T}$ is *unbounded* on the Hilbert space \mathcal{H}_{TV} , as discussed in Section E. It is therefore natural to start our discussion with a more detailed look into this distinction, in the present context. Since $\mathbf{\Gamma}$ is an orthogonal projector from \mathcal{H}_V to \mathcal{H}_\times , it is bounded by unity in operator norm $\|\mathbf{\Gamma}\| \leq 1$ on \mathcal{H}_V and $\|\mathbf{\Gamma}\| = 1$ on \mathcal{H}_\times [79, 87]. Therefore by (E.3), in the case of steady flows, the operator $\mathbf{A} = \mathbf{\Gamma} \mathbf{H} \mathbf{\Gamma}$ is bounded on the Hilbert space \mathcal{H}_V , with $\|\mathbf{A}\| \leq \|\mathbf{H}\| < \infty$. Let's first focus on this time-independent case. Since $\mathbf{M} = -\iota \mathbf{A}$ we have $\|\mathbf{M}\| = \|\mathbf{A}\|$, so the domains of these two operators are identical, $D(\mathbf{M}) = D(\mathbf{A})$. For simplicity we focus on the operator \mathbf{M} now, re-introducing the operator \mathbf{A} later. The (Hilbert space) adjoint \mathbf{M}^* of \mathbf{M} is defined by $\langle \mathbf{M} \boldsymbol{\psi}, \boldsymbol{\varphi} \rangle = \langle \boldsymbol{\psi}, \mathbf{M}^* \boldsymbol{\varphi} \rangle$, and is also a bounded operator on \mathcal{H}_V with $\|\mathbf{M}^*\| = \|\mathbf{M}\|$ [79]. Consequently, they have identical domains,

$$(F.1) \quad D(\mathbf{M}) = D(\mathbf{M}^*),$$

which are the entire space, $D(\mathbf{M}) = D(\mathbf{M}^*) = \mathcal{H}_V$. In Section F.4 we show that \mathbf{M} is symmetric,

$$(F.2) \quad \langle \mathbf{M} \boldsymbol{\psi} \cdot \boldsymbol{\varphi} \rangle = \langle \boldsymbol{\psi} \cdot \mathbf{M} \boldsymbol{\varphi} \rangle, \text{ for all } \boldsymbol{\psi}, \boldsymbol{\varphi} \in D(\mathbf{M}).$$

By definition [79, 87], the two properties (A.1) and (A.2) together imply that the operator \mathbf{M} is *self-adjoint*, i.e. $\mathbf{M} \equiv \mathbf{M}^*$ on $D(\mathbf{M})$.

As $\mathbf{\Gamma}$ is bounded on $\mathcal{H}_{\mathcal{V}}$ and $\mathbf{M} = -\imath \mathbf{\Gamma} \mathbf{S} \mathbf{\Gamma}$, our discussion in Section E indicates that the unboundedness of \mathbf{M} on $\mathcal{H}_{\mathcal{TV}}$ is due to the unboundedness of the underlying operator \mathbf{T} on the Hilbert space $\mathcal{H}_{\mathcal{T}}$. It is therefore necessary that we find a domain $D(\mathbf{T})$ for which $\imath \mathbf{T}$ is a self-adjoint operator.

The spectral theorem of equation (A.7) for the maximal normal operator \mathbf{N} on \mathcal{F} generalizes that for self-adjoint and maximal anti-symmetric operators, with purely real and imaginary spectrum, respectively. More specifically, the case $F(z) = z = \lambda_1 + \imath \lambda_2$ corresponds to $F(\mathbf{N}) = \mathbf{H}_1 + \imath \mathbf{H}_2$ with $I \subseteq (-\infty, \infty) \times (-\imath \infty, \imath \infty)$ and $\mathbf{Q}(z) = \mathbf{Q}_1(\text{Re}(z))\mathbf{Q}_2(\text{Im}(z))$, the case $F(z) = \text{Re}(z)$ corresponds to the self-adjoint operator $F(\mathbf{N}) = \mathbf{H}_1$ with $I \subseteq (-\infty, \infty)$ and $\mathbf{Q}(z) = \mathbf{Q}_1(\text{Re}(z))$, and the case $F(z) = \imath \text{Im}(z)$ corresponds to the maximal anti-symmetric operator $F(\mathbf{N}) = \imath \mathbf{H}_2$ with $I \subseteq (-\imath \infty, \imath \infty)$ and $\mathbf{Q}(z) = \mathbf{Q}_2(\text{Im}(z))$ [87]. We now apply the spectral theorem to equations (C.20) and (E.9) to provide Radon–Stieltjes integral representations for the symmetric \mathbf{D}^* and anti-symmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* , for both cases of time-independent and time-dependent velocity fields \mathbf{u} . These representations are summarized by the following theorem.

THEOREM F.1. *Let $z = \imath \lambda$, $\mathbf{g}_j = -\mathbf{\Gamma} \mathbf{H} \mathbf{e}_j$ be defined as in (E.9), and $\mathbf{Q}(z) = \mathbf{Q}_2(\text{Im}(z)) = \mathbf{Q}_2(\lambda)$ be the complex resolution of the identity associated with the maximal anti-symmetric operator \mathbf{A} defined in (E.9), with domain \mathcal{F} defined in (E.4). Define the matrix-valued function $\boldsymbol{\mu}(\lambda)$ with complex-valued off-diagonal components $\mu_{jk}(\lambda) = \langle \mathbf{Q}_2(\lambda) \mathbf{g}_j \cdot \mathbf{g}_k \rangle$ for $j \neq k = 1, \dots, d$, with $\mu_{kj} = \bar{\mu}_{jk}$, and positive diagonal components $\mu_{kk}(\lambda) = \|\mathbf{Q}_2(\lambda) \mathbf{g}_k\|^2$. Moreover, consider the real-valued functions*

$$(F.3) \quad \text{Re } \mu_{jk}(\lambda) = \frac{1}{2} (\mu_{jk}(\lambda) + \bar{\mu}_{jk}(\lambda)), \quad \text{Im } \mu_{jk}(\lambda) = \frac{1}{2\imath} (\mu_{jk}(\lambda) - \bar{\mu}_{jk}(\lambda)).$$

Corresponding to each of these functions of bounded variation, consider the associated Radon–Stieltjes measures $d\mu_{jk}(\lambda)$, $d\mu_{kk}(\lambda)$, $d\text{Re } \mu_{jk}(\lambda)$, and $d\text{Im } \mu_{jk}(\lambda)$. Then, for all $0 < \varepsilon < \infty$, there exist Radon–Stieltjes integral representations for the components \mathbf{S}_{jk}^ and \mathbf{A}_{jk}^* , $j, k = 1, \dots, d$, of the effective tensors \mathbf{D}^* and \mathbf{A}^* defined in equation (C.20), given by*

$$(F.4) \quad \mathbf{S}_{jk}^* = \varepsilon \left(\delta_{jk} + \int_{-\infty}^{\infty} \frac{d\text{Re } \mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2} \right), \quad \mathbf{A}_{jk}^* = \int_{-\infty}^{\infty} \frac{\lambda d\text{Im } \mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2}.$$

Here, the domain of integration I is determined by the spectrum $\Sigma(\mathbf{A})$ of the operator \mathbf{A} , where $I \subseteq [-\|\mathbf{A}\|, \|\mathbf{A}\|]$ and $\|\mathbf{A}\| \leq \|\mathbf{H}\| < \infty$ in the case of a time-independent velocity field \mathbf{u} [79].

A key feature of the integral representations for \mathbf{D}^* and \mathbf{A}^* in (2.14) is that parameter information in ε is *separated* from the geometry and dynamics of the velocity field \mathbf{u} , which are encapsulated in the underlying spectral measure $d\boldsymbol{\mu}$. In Section F.7 we will discuss in more detail the properties of the spectrum $\Sigma(\mathbf{A})$ of the operator \mathbf{A} . Moreover, we show how these properties of Σ lead to useful decompositions of the measure $d\boldsymbol{\mu}$. These measure decompositions are employed in Section 3 to calculate \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* for a large class of velocity fields \mathbf{u} . Furthermore, in Section ?? these important properties of the integrals in (2.14) lead to asymptotic behavior of \mathbf{D}^* and \mathbf{A}^* in the advection and diffusion dominated regimes, where the molecular diffusivity tends to zero, $\varepsilon \rightarrow 0$, and infinity, $\varepsilon \rightarrow \infty$, respectively.

Proof of Theorem C.1. We first note that from $\nabla \chi_k \in \mathcal{F}$ we have $\nabla \chi_k = \mathbf{\Gamma} \nabla \chi_k$, so that \mathbf{A}_{jk}^* in equation (C.20) can re-expressed as $\mathbf{A}_{jk}^* = \langle \mathbf{S} \nabla \chi_j \cdot \nabla \chi_k \rangle = \langle \mathbf{\Gamma} \mathbf{S} \mathbf{\Gamma} \nabla \chi_j \cdot \nabla \chi_k \rangle = \langle \mathbf{A} \nabla \chi_j \cdot \nabla \chi_k \rangle$, where we have used that $\mathbf{\Gamma}$ is self-adjoint on \mathcal{F} . From this and (E.9), equation (C.20) can be rewritten as

$$(F.5) \quad \mathbf{S}_{jk}^* = \varepsilon (\delta_{jk} + \langle (\varepsilon \mathbf{I} + \mathbf{A})^{-1} \mathbf{g}_j \cdot (\varepsilon \mathbf{I} + \mathbf{A})^{-1} \mathbf{g}_k \rangle), \quad \mathbf{A}_{jk}^* = \langle \mathbf{A} (\varepsilon \mathbf{I} + \mathbf{A})^{-1} \mathbf{g}_j \cdot (\varepsilon \mathbf{I} + \mathbf{A})^{-1} \mathbf{g}_k \rangle,$$

where $\mathbf{g}_k = -\mathbf{\Gamma} \mathbf{H} \mathbf{e}_k$. The integral representations for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* in (2.14) follow from equations (A.7) and (F.5), and the symmetries $\langle \nabla \chi_j \cdot \nabla \chi_k \rangle = \langle \nabla \chi_k \cdot \nabla \chi_j \rangle$ and $\langle \mathbf{A} \nabla \chi_j \cdot \nabla \chi_k \rangle = \langle \nabla \chi_k \cdot \mathbf{A} \nabla \chi_j \rangle$, since $\nabla \chi_k$ and $\mathbf{A} \nabla \chi_k$ are real-valued. We prove the validity of (2.14) by showing that the conditions of the spectral theorem of equation (A.7) are satisfied for the functionals in (F.5) and then employing these symmetries.

We first show that $\mathbf{g}_k \in \mathcal{F}$ for all $k = 1, \dots, d$. Indeed, the orthogonality of the projection operators $\mathbf{\Gamma}_{\times} = \mathbf{\Gamma}$ and $\mathbf{\Gamma}_0$ defined in equation (C.10) implies that the vector field $\mathbf{g}_k(t, \cdot) = \mathbf{\Gamma} \mathbf{H}(t, \cdot) \mathbf{e}_k$ is curl-free and mean-zero for each $t \in \mathcal{T}$ fixed, and by equation (E.3) we have $\|\mathbf{g}_k\| \leq \|\mathbf{H}\| < \infty$. This and the periodicity of \mathbf{H} implies that $\mathbf{g}_k(t, \cdot) \in \mathcal{H}_{\times}$, and by Fubini's theorem [33] we have $\langle \mathbf{g}_k \rangle = 0$. By the uniform boundedness of $\mathbf{\Gamma}$ on $\mathcal{H}_{\mathcal{V}}$ and equation (E.3), we also have [33] that $\|\mathbf{T} \mathbf{g}_k\| = \|\mathbf{T} \mathbf{\Gamma} \mathbf{H} \mathbf{e}_k\| = \|\mathbf{\Gamma} \mathbf{T} \mathbf{H} \mathbf{e}_k\| \leq \|\mathbf{T} \mathbf{H}\| < \infty$.

Therefore $\mathbf{g}_k(\cdot, \mathbf{x}), \mathbf{T}\mathbf{g}_k(\cdot, \mathbf{x}) \in \mathcal{H}_{\mathcal{T}}$ for each $\mathbf{x} \in \mathcal{V}$ fixed, which implies that $\mathbf{g}_k(\cdot, \mathbf{x}) \in \mathcal{F}_{\mathcal{T}}$. Consequently, $\mathbf{g}_k \in \mathcal{F}$ for all $k = 1, \dots, d$.

Consider the representation for \mathbf{S}_{jk}^* in (F.5) and define the function $F(z) = (\varepsilon + z)^{-1}$ so that, formally, $\mathbf{S}_{jk}^* = \varepsilon(\delta_{jk} + \langle F(\mathbf{A})\mathbf{g}_j \cdot F(\mathbf{A})\mathbf{g}_k \rangle)$. Since $\mathbf{g}_k \in \mathcal{F}$ for all $k = 1, \dots, d$, once we establish that $\mathbf{g}_k \in \mathcal{D}(F)$, i.e. $F \in L^2(\mu_{kk})$, the integral representations for \mathbf{S}_{jk}^* , $j, k = 1, \dots, d$, in (2.14) follow from the second formula in (A.7) with $F(z) = G(z) = (\varepsilon + z)^{-1}$, $\psi = \mathbf{g}_j$, and $\varphi = \mathbf{g}_k$. Since $0 < \varepsilon < \infty$ and $z \in (-i\infty, i\infty)$ for the anti-symmetric operator \mathbf{A} , the function $|F(z)|^2 = |\varepsilon + z|^{-2}$ is bounded, and the validity of $F \in L^2(\mu_{kk})$ is an immediate consequence of the boundedness of the (positive) measure mass $\mu_{kk}^0 = \int d\mu_{kk}(z) < \infty$. The validity of $\mu_{kk}^0 < \infty$, in turn, is a consequence of the fact that the function $\mu_{jk}(z) = \langle \mathbf{Q}(z)\mathbf{g}_j \cdot \mathbf{g}_k \rangle$ is of bounded variation when $\mathbf{g}_j, \mathbf{g}_k \in \mathcal{F}$, hence $|\mu_{jk}^0| < \infty$ for all $j, k = 1, \dots, d$ [87]. We have therefore established that $\mathbf{g}_k \in \mathcal{D}(F)$ for all $k = 1, \dots, d$.

The self-adjointness of $\mathbf{\Gamma}$ and $\mathbf{\Gamma}^2 = \mathbf{\Gamma}$ on \mathcal{F} implies that

$$(F.6) \quad \mu_{jk}^0 = \int_{-\infty}^{\infty} d\langle \mathbf{Q}(z)\mathbf{g}_j, \mathbf{g}_k \rangle = \langle \mathbf{g}_j, \mathbf{g}_k \rangle = \langle \mathbf{\Gamma}\mathbf{H}\mathbf{e}_j \cdot \mathbf{\Gamma}\mathbf{H}\mathbf{e}_k \rangle = \langle \mathbf{H}^T \mathbf{\Gamma}\mathbf{H}\mathbf{e}_j \cdot \mathbf{e}_k \rangle.$$

This and equation (E.3) imply that $|\mu_{jk}^0| \leq \|\mathbf{H}\|^2 < \infty$ for all $j, k = 1, \dots, d$.

This concludes our proof of Theorem C.1 \square .

F.2. An isometric correspondence. A natural question to ask is the following. Is the formulation of the effective parameter problem described in Theorem C.3 equivalent to that described in Corollary ??? The correspondence between the two formulations is one of isometry, and is summarized by the following theorem.

THEOREM F.2. *The function spaces \mathcal{F} and \mathcal{F} defined in equations (E.4) and (C.3) are in one-to-one isometric correspondence. This induces a one-to-one isometric correspondence between the domains $D(\mathbf{A})$ and $D(A)$ of the operators \mathbf{A} and A defined in equations (E.9) and (2.11), respectively. Specifically, for every $f \in D(A)$ we have $\nabla f \in D(\mathbf{A})$ and $\|\mathbf{A}f\|_1 = \|\mathbf{A}\nabla f\|$, and conversely, for each $\psi \in D(\mathbf{A})$ there exists unique $f \in D(A)$ such that $\psi = \nabla f$ and $\|\mathbf{A}\psi\| = \|\mathbf{A}f\|_1$. The Radon–Stieltjes measures underlying the integral representations of Theorem C.3 and Corollary ?? are equal, $d\langle \mathbf{Q}_2(\lambda)\mathbf{g}_j, \mathbf{g}_k \rangle_1 = d\langle \mathbf{Q}_2(\lambda)\mathbf{g}_j, \mathbf{g}_k \rangle$, $j, k = 1, \dots, d$, up to null sets of measure zero, where $\mathbf{g}_j = \nabla g_j$. Moreover, the operators \mathbf{A} and A are related by $\mathbf{A}\nabla = \nabla A$, which implies and is implied by the weak equality $\mathbf{Q}_2(\lambda)\nabla = \nabla \mathbf{Q}_2(\lambda)$.*

Proof of Theorem F.2. We use the formula $\mathbf{u} = \nabla \cdot \mathbf{H}$ displayed in equation (C.12) to write the operator $A = \Delta^{-1}(\mathbf{u} \cdot \nabla - \partial_t)$ and function $g_j = (-\Delta)^{-1}u_j$ defined in equations (2.11) and (2.12) as $A = \Delta^{-1}(\nabla \cdot \mathbf{H}\nabla - \partial_t)$ and $g_j = (-\Delta)^{-1}\nabla \cdot \mathbf{H}\mathbf{e}_j$, respectively. Using the definition $\mathbf{\Gamma} = \nabla(\Delta^{-1})\nabla \cdot$ and the formulas $\nabla\Delta^{-1}\partial_t = \Delta^{-1}\mathbf{T}\nabla$, $\mathbf{g}_j = -\mathbf{\Gamma}\mathbf{H}\mathbf{e}_j$, and $\mathbf{A} = \mathbf{\Gamma}\mathbf{H} - \Delta^{-1}\mathbf{T}$ displayed in equations, (E.9), and (E.10), respectively, we have that

$$(F.7) \quad \nabla A = [\mathbf{\Gamma}\mathbf{H} - \Delta^{-1}\mathbf{T}]\nabla = \mathbf{A}\nabla, \quad \nabla g_j = \mathbf{g}_j.$$

Consequently, by applying the differential operator ∇ to both sides of the formula $(\varepsilon + A)\chi_j = g_j$ of (2.12), we obtain the formula $(\varepsilon\mathbf{I} + \mathbf{A})\nabla\chi_j = \mathbf{g}_j$ of equation (E.9).

Since the function spaces \mathcal{F} and \mathcal{F} differ only in the characterization of the spatial variable \mathbf{x} , we now discuss the relationship between the Hilbert spaces $\mathcal{H}_{\mathbf{x}}$ and $\mathcal{H}_{\mathcal{V}}^1$ defined in equations (C.10) and (C.2), respectively, with inner-product induced norms $\|\cdot\|$ and $\|\cdot\|_1$. For $f \in \mathcal{H}_{\mathcal{V}}^1 \subset L^2(\mathcal{V})$ we have $\Delta^{-1}\Delta f = f$ [85], which implies that $\mathbf{\Gamma}\nabla f = \nabla f$ and $\|\nabla f\|^2 = \langle \nabla f \cdot \nabla f \rangle = \|f\|_1^2 < \infty$. Consequently, for every $f \in \mathcal{H}_{\mathcal{V}}^1$ we have $\nabla f \in \mathcal{H}_{\mathbf{x}}$. Conversely, $\psi \in \mathcal{H}_{\mathbf{x}}$ implies that $\psi = \mathbf{\Gamma}\psi = \nabla f$, where we have defined the scalar-valued function $f = \Delta^{-1}\nabla \cdot \psi$. Since $\psi = \nabla f$, the $\mathcal{H}_{\mathcal{V}}^1$ norm of f satisfies $\|f\|_1^2 = \langle \psi \cdot \psi \rangle = \|\psi\|^2 < \infty$ so that $f \in \mathcal{H}_{\mathcal{V}}^1$. Moreover, f is uniquely determined by ψ up to equivalence class, since if $f_1 = \Delta^{-1}\nabla \cdot \psi$ and $f_2 = \Delta^{-1}\nabla \cdot \psi$ then $\mathbf{\Gamma}\psi = \psi$ implies that $\|f_1 - f_2\|_1 = \|\psi - \psi\| = 0$. Consequently, for every $\psi \in \mathcal{H}_{\mathbf{x}}$ there exists unique $f \in \mathcal{H}_{\mathcal{V}}^1$ such that $\psi = \nabla f$. In summary, the Hilbert spaces $\mathcal{H}_{\mathcal{V}}^1$ and $\mathcal{H}_{\mathbf{x}}$ are in one-to-one isometric correspondence, which we denote by $\mathcal{H}_{\mathcal{V}}^1 \sim \mathcal{H}_{\mathbf{x}}$. This, in turn, implies $\mathcal{F} \sim \mathcal{F}$.

We now return to our previous notation, where $\|\cdot\|_1$ and $\|\cdot\|$ denotes the norm induced by the \mathcal{F} - and \mathcal{F} -inner-product, respectively. We demonstrate that the one-to-one isometry between \mathcal{F} and \mathcal{F} induces a one-to-one isometry between the domains $D(A)$ and $D(\mathbf{A})$ of the operators A and \mathbf{A} , i.e. $D(A) \sim D(\mathbf{A})$. This, in turn, follows from another on-to-one isometry between the class of self-adjoint operators on \mathcal{F} ,

for example, and the class of resolutions of the identity. This correspondence is determined directly as follows [87]. Let X be a self-adjoint operator on \mathcal{F} and $Q(\lambda)$ be the associated resolution of the identity, which is a one-to-one correspondence [87]. The domain $D(X)$ of X comprises those and only those elements $f \in \mathcal{F}$ such that the Stieltjes integral $\int_{-\infty}^{\infty} \lambda^2 d\|Q(\lambda)f\|_1^2$ is convergent; when $f \in D(X)$ the element Xf is determined by the relations

$$(F.8) \quad \langle Xf, h \rangle_1 = \int_{-\infty}^{\infty} \lambda d\langle Q(\lambda)f, h \rangle_1, \quad \|Xf\|_1^2 = \int_{-\infty}^{\infty} \lambda^2 d\|Q(\lambda)f\|_1^2,$$

where h is an arbitrary element in \mathcal{F} [87]. Since $M = -\imath A$ is self-adjoint on \mathcal{F} and $D(A) = D(M)$, this one-to-one isometric correspondence also holds for the maximal normal operator A , and a calculation similar to that in equations (??) and (??) shows that equation (A.11) holds under the mappings $X \mapsto A$, $\lambda d\langle Q(\lambda)f, h \rangle_1 \mapsto \lambda d\text{Im} \langle Q(\lambda)f, h \rangle_1$, and $Q(\lambda) \mapsto Q_2(\lambda)$. An analogous result holds for the self-adjoint operator $\mathbf{M} = -\imath \mathbf{A}$ on \mathcal{F} with $D(\mathbf{A}) = D(\mathbf{M})$.

We now demonstrate that the one-to-one isometry between the class of self-adjoint operators and resolutions of the identity on \mathcal{F} , and that for \mathcal{F} , along with the property $\mathcal{F} \sim \mathcal{F}$ and equation (F.7), induce the one-to-one isometry $D(A) \sim D(\mathbf{A})$. From $\mathcal{F} \sim \mathcal{F}$, we have for every $f \in D(A) \subset \mathcal{F}$ that $\nabla f \in \mathcal{F}$, so from equation (F.7)

$$(F.9) \quad \|Af\|_1^2 = \langle Af, Af \rangle_1 = \langle \nabla Af \cdot \nabla Af \rangle = \langle \mathbf{A} \nabla f \cdot \mathbf{A} \nabla f \rangle = \|\mathbf{A} \nabla f\|^2.$$

Consequently, from equation (A.11) we have

$$(F.10) \quad \int \lambda^2 d\|Q_2(\lambda)f\|_1^2 = \int \lambda^2 d\|\mathbf{Q}_2(\lambda)\nabla f\|^2,$$

and the convergence of the left-hand-side of (F.10) implies the convergence of the right-hand-side which, in turn, implies that $\nabla f \in D(\mathbf{A})$. Conversely, from $\mathcal{F} \sim \mathcal{F}$ we have that $\psi \in D(\mathbf{A}) \subset \mathcal{F}$ implies there exists unique $f \in \mathcal{F}$ such that $\psi = \nabla f$, and equation (F.7) then implies that

$$(F.11) \quad \|\mathbf{A}\psi\|^2 = \langle \mathbf{A}\nabla f, \mathbf{A}\nabla f \rangle = \langle \nabla Af, \nabla Af \rangle = \langle Af, Af \rangle_1 = \|Af\|_1^2.$$

Again, equation (A.11) implies that (F.10) holds, and the convergence of the right-hand-side of (F.10) implies the convergence of the left-hand-side which, in turn, implies that $f \in D(A)$. In summary, for every $f \in D(A)$ we have $\nabla f \in D(\mathbf{A})$ and $\|Af\|_1^2 = \|\mathbf{A}\nabla f\|^2$. Conversely, for each $\psi \in D(\mathbf{A})$ there exists unique $f \in D(A)$ such that $\psi = \nabla f$ and $\|\mathbf{A}\psi\|^2 = \|Af\|_1^2$. Consequently, the domains $D(\mathbf{A})$ and $D(A)$ are in one-to-one isometric correspondence, i.e. $D(\mathbf{A}) \sim D(A)$.

We now show that this result implies, and is implied by the weak equality $\nabla Q_2(\lambda) = \mathbf{Q}_2(\lambda)\nabla$, where $Q_2(\lambda)$ and $\mathbf{Q}_2(\lambda)$ are the resolutions of the identity associated with the operators A and \mathbf{A} , respectively. From equation (F.10) and the linearity properties of Radon–Stieltjes integrals [87], we have that

$$(F.12) \quad 0 = \int_{-\infty}^{\infty} \lambda^2 d(\|Q_2(\lambda)f\|_1^2 - \|\mathbf{Q}_2(\lambda)\nabla f\|^2) = \int_{-\infty}^{\infty} \lambda^2 d(\langle [\nabla Q_2(\lambda) - \mathbf{Q}_2(\lambda)\nabla]f \cdot \nabla f \rangle).$$

Equation (F.12) implies that for all $f \in D(A) \iff \nabla f \in D(\mathbf{A})$ we have $d\|Q_2(\lambda)f\|_1^2 = d\|\mathbf{Q}_2(\lambda)\nabla f\|^2$, up to null sets of measure zero. Moreover, the equality $\nabla Q_2(\lambda) = \mathbf{Q}_2(\lambda)\nabla$ holds weakly. Conversely, assume that $Q_2(\lambda)$ and $\mathbf{Q}_2(\lambda)$ are the resolutions of the identity associated with the operators A and \mathbf{A} on the function spaces \mathcal{F} and \mathcal{F} , respectively, which is a one-to-one correspondence [87], and that $\nabla Q_2(\lambda)f = \mathbf{Q}_2(\lambda)\nabla f$ holds for every $f \in D(A) \iff \nabla f \in D(\mathbf{A})$. Then equation (F.12) holds and implies equation (F.10). The correspondence $D(A) \sim D(\mathbf{A})$ and equation (A.11) then imply that $\|\mathbf{A}\nabla f\|^2 = \|Af\|_1^2 = \|\nabla Af\|^2$, hence $\|(\mathbf{A}\nabla - \nabla A)f\|^2 = 0$ for every $f \in D(A) \iff \nabla f \in D(\mathbf{A})$, which implies that $\mathbf{A}\nabla = \nabla A$ weakly. Since $g_k \in D(A)$ and $\mathbf{g}_k \in D(\mathbf{A})$ with $\mathbf{g}_k = \nabla g_k$, this result implies that the Radon–Stieltjes measures underlying the integral representations of Theorem C.3 and Corollary ?? are equal $d\langle Q_2(\lambda)g_j, g_k \rangle_1 = d\langle \mathbf{Q}_2(\lambda)\mathbf{g}_j, \mathbf{g}_k \rangle$ up to null sets of measure zero, for all $j, k = 1, \dots, d$. This concludes our proof of Theorem F.2 \square .

F.3. Section Break Here. In Section C we provide two natural Hilbert space formulations of the effective parameter problem for advection enhanced diffusion, yielding integral representations for both the symmetric and antisymmetric parts of the effective diffusivity tensor \mathbf{D}^* . This approach is based on the spectral theorem discussed in this section and resolvent formulas for the functions $\nabla\chi_j$ and χ_j , introduced in equations (2.9) and (2.8), involving self-adjoint operators on appropriate Hilbert spaces. In Section F.2 we prove that the two formulations are equivalent, and follow from an one-to-one isometric correspondence between the underlying Hilbert spaces and the one-to-one correspondence between the operator and its resolution of the identity determined by equation (A.11). FINISH THIS PARAGRAPH AFTER SECTION C IS WRITTEN.

F.4. Antisymmetry. In this section we show that the operator $A = (-\Delta)^{-1}(\partial_t - \mathbf{u} \cdot \nabla)$ defined in equation (2.11) is *antisymmetric* on the function space \mathcal{F} defined in (C.3). We first show that the incompressibility condition $\nabla \cdot \mathbf{u} = 0$ implies that the operator $(\Delta^{-1})(\mathbf{u} \cdot \nabla)$ is antisymmetric [12] on the Sobolev space \mathcal{H}_V^1 defined in equation (C.2). Indeed, since $\Delta = \nabla \cdot \nabla$ and (Δ^{-1}) is self-adjoint [85] on \mathcal{H}_V^1 , for $f, h \in \mathcal{H}_V^1$ we have

$$\begin{aligned}
 \langle (\Delta^{-1})(\mathbf{u} \cdot \nabla)f, h \rangle_1 &= \langle [\nabla(\Delta^{-1})(\mathbf{u} \cdot \nabla)f] \cdot \nabla h \rangle \\
 &= -\langle [(\mathbf{u} \cdot \nabla)f] h \rangle \\
 &= -\langle [\nabla \cdot (\mathbf{u}f)] h \rangle \\
 &= \langle f [(\mathbf{u} \cdot \nabla)h] \rangle \\
 &= \langle (\Delta^{-1})\Delta f [(\mathbf{u} \cdot \nabla)h] \rangle \\
 &= -\langle \nabla f \cdot \nabla [(\Delta^{-1})(\mathbf{u} \cdot \nabla)h] \rangle \\
 &= -\langle f, (\Delta^{-1})(\mathbf{u} \cdot \nabla)h \rangle_1.
 \end{aligned}
 \tag{F.13}$$

We now show that the operator $(-\Delta)^{-1}\partial_t$ is skew-adjoint on \mathcal{F} . For $f \in \mathcal{F}$ we have $f(\cdot, \mathbf{x}) \in \tilde{\mathcal{A}}_T$ for all $\mathbf{x} \in \mathcal{V}$ and $f(t, \cdot) \in \mathcal{H}_V^1$ for every $t \in \mathcal{T}$. Moreover, since $\mathcal{H}_V^1 \subset L^2(\mathcal{V})$ and $(-\Delta)^{-1}$ is a bounded Hilbert-Schmidt integral operator on $L^2(\mathcal{V})$ [85], Theorem 2.27 of [33] establishes that the operators $(-\Delta)^{-1}$ and ∂_t commute on \mathcal{F} . Consequently, since $(-\Delta)^{-1}$ is self-adjoint on $L^2(\mathcal{V})$ and ∂_t is skew-adjoint on $\tilde{\mathcal{A}}_T$, the operator $(-\Delta)^{-1}\partial_t$ is skew-adjoint on \mathcal{F} . It follows that the operator $A = (-\Delta)^{-1}(\partial_t - \mathbf{u} \cdot \nabla)$ is *antisymmetric* on \mathcal{F} \square .

F.5. Multiple scale method. In this section we provide the details of the multiple scale method [60, 69, 70, 8] which leads to equations (2.3)–(C.20). We assume that equation (2.1) has already been non-dimensionalized so that $\kappa_0 \mapsto \varepsilon$ and $\mathbf{u} \mapsto \mathbf{u}$. The key assumption of the method is that the initial density ϕ_0 in (2.1) is slowly varying relative to the velocity field \mathbf{u} , which introduces a small parameter $\delta \ll 1$ such that

$$(F.14) \quad \phi(0, \mathbf{x}) = \phi_0(\delta \mathbf{x}).$$

The variable changes $\mathbf{x} \mapsto \mathbf{y} = \mathbf{x}/\delta$ and $t \mapsto \tau = t/\delta^2$, along with equations (??) and (F.14), transforms equation (2.1) into [60]

$$(F.15) \quad \partial_t \phi^\delta(t, \mathbf{x}) = \varepsilon \Delta \phi^\delta(t, \mathbf{x}) + \delta^{-1} \mathbf{u}(\tau, \mathbf{y}) \cdot \nabla \phi^\delta(t, \mathbf{x}), \quad \phi^\delta(0, \mathbf{x}) = \phi_0(\mathbf{x}).$$

We now expand ϕ^δ in powers of δ [60]

$$(F.16) \quad \phi^\delta(t, \mathbf{x}) = \bar{\phi}(t, \mathbf{x}) + \delta \phi^{(1)}(t, \mathbf{x}, \tau, \mathbf{y}) + \delta^2 \phi^{(2)}(t, \mathbf{x}, \tau, \mathbf{y}) + \dots$$

Writing

$$\partial_t \phi^{(n)} = [\partial_t + \delta^{-2} \partial_\tau] \phi^{(n)}, \quad \nabla \phi^{(n)} = [\nabla_x + \delta^{-1} \nabla_y] \phi^{(n)}, \quad \Delta \phi^{(n)} = [\Delta_x + 2\delta^{-1} \nabla_x \cdot \nabla_y + \delta^{-2} \Delta_y] \phi^{(n)},$$

for the functions $\phi^{(i)}$, $n = 1, 2, \dots$, of the fast (τ, \mathbf{y}) and slow (t, \mathbf{x}) variables, we find that

$$(F.17) \quad \begin{aligned} \partial_t \phi^\delta &= \delta^{-2} [\partial_\tau \bar{\phi}] + \delta^{-1} [\partial_\tau \phi^{(1)}] + \delta^0 [\partial_t \bar{\phi} + \partial_\tau \phi^{(2)}] + O(\delta), \\ \nabla \phi^\delta &= \delta^{-2} [0] + \delta^{-1} [\nabla_y \bar{\phi}] + \delta^0 [\nabla_x \bar{\phi} + \nabla_y \phi^{(1)}] + \delta^1 [\nabla_x \phi^{(1)} + \nabla_y \phi^{(2)}] + O(\delta^2), \\ \Delta \phi^\delta &= \delta^{-2} [\Delta_y \bar{\phi}] + \delta^{-1} [2\nabla_x \cdot \nabla_y \bar{\phi} + \Delta_y \phi^{(1)}] + \delta^0 [\Delta_x \bar{\phi} + 2\nabla_x \cdot \nabla_y \phi^{(1)} + \Delta_y \phi^{(2)}] + O(\delta). \end{aligned}$$

Inserting this into equation (2.6) and setting the coefficients associated with the various powers of δ to zero, yields a sequence of problems.

Due to the dependence of $\bar{\phi}(t, \mathbf{x})$ on only the slow variables, the coefficients of δ^{-2} vanish. Equating the coefficients of δ^{-1} and δ^0 to zero we, respectively, obtain

$$(F.18) \quad \partial_\tau \phi^{(1)} - \varepsilon \Delta_y \phi^{(1)} - \mathbf{u} \cdot \nabla_y \phi^{(1)} = \mathbf{u} \cdot \nabla_x \bar{\phi},$$

$$(F.19) \quad \partial_\tau \phi^{(2)} - \mathbf{u} \cdot \nabla_y \phi^{(2)} - \varepsilon \Delta_y \phi^{(2)} = -\partial_t \bar{\phi} + \mathbf{u} \cdot \nabla_x \phi^{(1)} + \varepsilon [\Delta_x \bar{\phi} + 2\nabla_x \cdot \nabla_y \phi^{(1)}].$$

By the linearity of equation (F.18), we may separate the fast and slow variables by writing [60]

$$(F.20) \quad \phi^{(1)}(t, \mathbf{x}, \tau, \mathbf{y}) = \chi(\tau, \mathbf{y}) \cdot \nabla_x \bar{\phi}(t, \mathbf{x}).$$

When the components χ_k , $k = 1, \dots, d$, of χ satisfy the “cell problem”

$$(F.21) \quad \partial_\tau \chi_k - \varepsilon \Delta_y \chi_k - \mathbf{u} \cdot \nabla_y \chi_k = \mathbf{u} \cdot \mathbf{e}_k,$$

equation (F.18) is automatically satisfied [60]. Equation (F.21) along with (C.12) is equivalent to the cell problem (C.21), where the distinction of fast variables was dropped for notational simplicity. In order for $\phi^{(1)}(t, \mathbf{x}, \tau, \mathbf{y})$ in (F.20) to be periodic in (τ, \mathbf{y}) for each fixed (t, \mathbf{x}) , we must have that the functions $\chi_k(\tau, \mathbf{y})$, $k = 1, \dots, d$, are periodic. This and the fundamental theorem of calculus implies that $\langle \nabla_y \chi_k \rangle = 0$. Here, $\langle \cdot \rangle$ denotes space-time averaging with respect to the *fast variables*.

Due to the incompressibility of the velocity field $\nabla_y \cdot \mathbf{u}(\tau, \mathbf{y}) = 0$ and the *a priori* fast variable periodicity of the functions $\phi^{(i)}$, $i = 1, 2$, the fundamental theorem of calculus and the divergence theorem shows that the average of the left-hand-sides of equations (F.18) and (F.19) are zero. For the equations to have solutions, the average of the right-hand-sides must also vanish. The resulting solvability conditions are $\langle \mathbf{u} \rangle = 0$ and the following equation which governs the large-scale (slow variable) dynamics

$$(F.22) \quad \partial_t \bar{\phi} = \varepsilon \Delta_x \bar{\phi} + \langle \mathbf{u} \cdot \nabla_x \phi^{(1)} \rangle.$$

Here, we have used that $\bar{\phi}$ is a *constant* with respect to the fast variables and, by the divergence theorem and the fast variable periodicity of $\phi^{(1)}$, we have $\langle \nabla_y \cdot \nabla_x \phi^{(1)} \rangle = 0$. The convergence of ϕ^δ to $\bar{\phi}$ as $\delta \rightarrow 0$ is in L^2 [28],

$$(F.23) \quad \lim_{\delta \rightarrow 0} \left[\sup_{0 \leq t \leq t_0} \int |\phi^\delta(t, \mathbf{x}) - \bar{\phi}(t, \mathbf{x})|^2 d\mathbf{x} \right] = 0,$$

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

Inserting equation (F.20) into (F.22) yields equation (2.3) with the components $D_{jk}^* = D^* \mathbf{e}_j \cdot \mathbf{e}_k$ of the effective diffusivity tensor D^* given by

$$(F.24) \quad D_{jk}^* = \varepsilon \delta_{jk} + \langle u_j \chi_k \rangle.$$

By inserting the representation for u_j in (F.21) into equation (F.24), the functional $\langle u_j \chi_k \rangle$ can be represented in terms of $\nabla_y \chi_j$ and the *skew-symmetric* operator $\mathbf{S} = \mathbf{H} + (-\Delta_y)^{-1} \mathbf{T}$, where the inverse operation $(-\Delta_y)^{-1}$ is based on convolution with the Green's function for the Laplacian Δ_y , $\mathbf{T} = \partial_\tau \mathbf{l}$, and the \mathbf{l} in this definition is to remind us that the derivative ∂_τ operates component-wise. Indeed, writing $\partial_\tau \chi_j = \nabla_y \cdot (\Delta_y^{-1} \mathbf{T}) \nabla_y \chi_j$, $\Delta_y \chi_j = \nabla_y \cdot \nabla_y \chi_j$, and $\mathbf{u} = \nabla_y \cdot \mathbf{H}$ in (C.12), we have

$$(F.25) \quad \begin{aligned} \langle u_j \chi_k \rangle &= \langle [\partial_\tau \chi_j - \varepsilon \Delta_y \chi_j - \mathbf{u} \cdot \nabla_y \chi_j] \chi_k \rangle \\ &= \langle \nabla_y \cdot [(\Delta_y^{-1} \mathbf{T} - \varepsilon \mathbf{l} - \mathbf{H}) \nabla_y \chi_j] \chi_k \rangle \\ &= \langle [(\mathbf{H} + (-\Delta_y)^{-1} \mathbf{T} + \varepsilon \mathbf{l}) \nabla_y \chi_j] \cdot \nabla_y \chi_k \rangle \\ &= \langle \mathbf{S} \nabla_y \chi_j \cdot \nabla_y \chi_k \rangle + \varepsilon \langle \nabla_y \chi_j \cdot \nabla_y \chi_k \rangle, \end{aligned}$$

where we have used the periodicity of χ_k and \mathbf{H} to obtain the third equality. Equations (F.24) and (C.23) are equivalent to equations (2.10) and (C.20), where the distinction of fast variables was dropped for notational simplicity.

The above analysis shows that the main part of the study of effective, diffusive transport enhanced by periodic, incompressible flows, is the study of equation (F.21), from which the effective diffusivity tensor D^* emerges. In Section E, we use the analytical structure of the cell problem (F.21) to derive a resolvent representation for $\nabla_y \chi_k$, involving an anti-symmetric integro-differential operator \mathbf{A} which is related to $\mathbf{S} = \mathbf{H} - \Delta^{-1} \partial_t \mathbf{l}$. In Section F, we employ this representation for $\nabla_y \chi_k$ and the spectral theorem, to provide integral representations for D^* and A^* involving a *spectral measure* associated with the operator \mathbf{A} acting on a suitable Hilbert space.

F.6. Existence and Uniqueness. THIS SECTION IS UNDER CONSTRUCTION

Before we discuss how the Hilbert space framework presented above leads to an integral representation for D^* , we first discuss some key differences in the theory between the cases of steady and dynamic velocity fields \mathbf{u} . These differences are reflected in the measure underlying this integral representation for D^* and stem from the *unboundedness* of the operator ∂_t on the Hilbert space \mathcal{H}_T [79, 87]. For steady \mathbf{u} , in general, equation (D.11) reduces to (C.20) for diagonal components of the effective parameter. However, for dynamic \mathbf{u} , this is not true in general. The details are as follows. For dynamic \mathbf{u} , the operator σ in (C.17) can be written as $\sigma = \varepsilon \mathbf{l} + \mathbf{S}$, where $\mathbf{S} = \mathbf{H} - \Delta^{-1} \partial_t \mathbf{l}$ is skew-symmetric $\langle \mathbf{S} \psi, \varphi \rangle = -\langle \psi, \mathbf{S} \varphi \rangle$ for all $\psi, \varphi \in \mathcal{F}$ such that $|\langle \partial_t \psi, \varphi \rangle|, |\langle \psi, \partial_t \varphi \rangle| < \infty$ (see Section ?? for details). This property of the operator \mathbf{S} implies that

$$(F.26) \quad \langle \mathbf{S} \psi \cdot \psi \rangle = -\langle \mathbf{S} \psi \cdot \psi \rangle = 0, \quad \mathbf{S} = \mathbf{H} - (\Delta^{-1}) \partial_t \mathbf{l},$$

for all such $\psi \in \mathcal{F}$. In this dynamic setting, equation (D.8) does not hold for every $\psi \in \mathcal{F}$, as the unbounded operator ∂_t is defined only on a proper (dense) subset of the Hilbert space \mathcal{H}_T [79], and it may be that $|\langle \partial_t \psi, \psi \rangle| = \infty$. In the case of a steady velocity field we have $\mathbf{S} \equiv \mathbf{H}$ and, by equation (E.3) and the Cauchy Schwartz inequality, $|\langle \mathbf{S} \psi, \psi \rangle| \leq \|\mathbf{H}\| \|\psi\|^2 < \infty$ for all $\psi \in \mathcal{F}$, so equation (D.8) holds for all $\psi \in \mathcal{F}$.

Another immediate consequence of equation (D.8), for steady \mathbf{u} , is the coercivity of the bilinear functional $\Phi(\psi, \varphi) = \langle \sigma \psi \cdot \varphi \rangle$ for all $\varepsilon > 0$. By equation (E.3), this functional is also bounded in the case of steady \mathbf{u} for all $\varepsilon < \infty$. Therefore, the Lax-Milgram theorem [62] provides the existence and uniqueness of a solution $\nabla \chi_k \in \mathcal{F}$ satisfying the cell problem (C.21), or equivalently equation (C.17), in this time-independent case. The details are as follows.

The distributional form of equation (C.21), written as $\nabla \cdot \sigma e_k = 0$, is given by $\langle \sigma(\nabla \chi_k + e_k) \cdot \nabla \varphi \rangle = 0$, where φ is a compactly supported, infinitely differentiable function on $\mathcal{T} \times \mathcal{V}$, and we stress that $\nabla \varphi$ is *curl-free*. Motivated by this, we consider the following variational problem: find $\nabla \chi_k \in \mathcal{F}$ such that

$$(F.27) \quad \langle \sigma(\nabla \chi_k + e_k) \cdot \psi \rangle = 0, \text{ for all } \psi \in \mathcal{F}.$$

In order to directly apply the Lax-Milgram Theorem, we rewrite equation (F.27) as

$$(F.28) \quad \Phi(\nabla \chi_k, \psi) = \langle \sigma \nabla \chi_k \cdot \psi \rangle = -\langle \sigma e_k \cdot \psi \rangle = f(\psi).$$

By equation (D.8) Φ is coercive, i.e.

$$(F.29) \quad \Phi(\psi, \psi) = \langle [(\varepsilon I + \mathbf{S})] \psi \cdot \psi \rangle = \varepsilon \|\psi\|^2 > 0, \text{ for all } \psi \in \mathcal{F}$$

such that $\|\psi\| \neq 0$ 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 (E.3), the triangle inequality, and the Cauchy-Schwartz inequality imply that Φ is also bounded for all $\varepsilon < \infty$

$$(F.30) \quad \Phi(\psi, \varphi) \leq (\varepsilon + \|\mathbf{H}\|) \|\psi\| \|\varphi\| < \infty, \text{ for all } \psi \in \mathcal{F}.$$

For the same reasons, the linear functional $f(\psi)$ in (F.28) is bounded for all $\psi \in \mathcal{F}$. Therefore, the Lax-Milgram theorem [62] provides the existence of a unique $\nabla \chi_k \in \mathcal{F}$ satisfying (C.21) in this time-independent case.

In the time-dependent case, equation (D.8) hence (F.29) does not hold for all $\psi \in \mathcal{F}$. Moreover, the operator ∂_t hence σ is not bounded on \mathcal{F} [79, 85], so (F.30) does not hold. Consequently, the Lax-Milgram theorem cannot be directly applied, and alternate techniques [34, 35] must be used to prove the existence and uniqueness of a solution $\nabla \chi_k \in \mathcal{F}$ satisfying the cell problem (C.21). This discussion illustrates key differences in the analytic structure of the effective parameter problem for \mathbf{D}^* , between the cases of steady and dynamic velocity fields \mathbf{u} , which stem from the unboundedness of the operator ∂_t on $\mathcal{H}_{\mathcal{T}}$, hence σ on \mathcal{F} . In Section F, 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 \mathbf{D}^* .

F.7. Discrete integral representations by eigenfunction expansion. The integral representations of Theorem C.1 and Corollary ?? for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* , displayed in equation (2.14), involve spectral measures $d\mu_{jk}(\lambda)$, $j, k = 1, \dots, d$, which have discrete and continuous components [79, 87]. In this section, we review these properties of $d\mu_{jk}(\lambda)$ and provide an explicit derivation of the discrete component of these integrals. The explicit representation of the underlying discrete measure will be used extensively in Section 3, which exploits Fourier methods to calculate \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* for a large class of velocity fields. This, in turn, provides numerical methods for the computation of \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* for such velocity fields, which will be exploited in Section 5.

We now summarize some general spectral properties of the maximal, anti-symmetric operators \mathbf{A} and A on the function spaces \mathcal{F} and \mathcal{F} defined in equations (E.4) and (C.3), respectively, which are dense subsets of their associated Hilbert spaces $\mathcal{H}_{\mathcal{X}}$ and \mathcal{H}^1 ,

$$(F.31) \quad \mathcal{H}_{\mathcal{X}} = \{\psi \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{X}} \mid \langle \psi \rangle = 0\}, \quad \mathcal{H}^1 = \{f \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1 \mid \langle f \rangle = 0\}.$$

See equations (C.9) and (C.1) for the notational definitions of equation (F.31). For simplicity, we focus on the operator A and the Hilbert space \mathcal{H}^1 , as the discussion regarding \mathbf{A} and $\mathcal{H}_{\mathcal{X}}$ is analogous.

Recall that the domain $D(A)$ of the maximal normal operator A comprises those and only those elements $f \in \mathcal{F}$ such that $\|Af\|_1^2 = \int_{-\infty}^{\infty} \lambda^2 d\|Q(\lambda)f\|_1^2 < \infty$, where $Q(\lambda)$ is the projection valued operator corresponding to A [87]. The integration is over the spectrum $\Sigma(A)$ of A , which has continuous Σ_{cont} and discrete (pure-point) Σ_{pp} components, $\Sigma(A) = \Sigma_{\text{cont}}(A) \cup \Sigma_{\text{pp}}(A)$. We first focus on the discrete spectrum $\Sigma_{\text{pp}}(A)$. The members $f \neq 0$ of $D(A)$ which satisfy $Af = v f$ with $v \in \Sigma_{\text{pp}}(A)$ are called eigenfunctions and v is the corresponding eigenvalue. The span of all eigenfunctions is a *countable* subspace of $D(A)$ [79, 87]. Accordingly, we will denote the eigenfunctions by φ_n , $n = 1, 2, \dots$, with corresponding eigenvalues v_n . Since

A is anti-symmetric, v_n is purely imaginary [87, 43] and we write $v_n = \imath\lambda_n$, where $\lambda_n \in \mathbb{R}$. Moreover, eigenfunctions corresponding to distinct eigenvalues are orthogonal and can be normalized to be orthonormal [87], i.e. if $A\varphi_n = v_n\varphi_n$, $A\varphi_m = v_m\varphi_m$, and $v_n \neq v_m$, then

$$(F.32) \quad \langle \varphi_n, \varphi_m \rangle_1 = \langle \nabla \varphi_n \cdot \nabla \varphi_m \rangle = \delta_{nm}.$$

There may be more than one eigenfunction associated with a particular eigenvalue. However, they are linearly independent and, without loss of generality, may be taken to be orthonormal [87]. Consequently, associated with each eigenfunction φ_n is a closed linear manifold, which we denote by $\mathcal{M}(\varphi_n)$. When $m \neq n$, $\mathcal{M}(\varphi_m)$ and $\mathcal{M}(\varphi_n)$ are mutually orthogonal. Set $\mathcal{E} = \bigoplus_{n=1}^{\infty} \mathcal{M}(\varphi_n)$, $\mathcal{M} = \mathcal{E} \oplus \{0\}$, and let $\mathcal{N} = \mathcal{M}^\perp$ be the orthogonal complement of \mathcal{M} in \mathcal{H}^1 .

The following theorem provides a natural decomposition of the Hilbert space \mathcal{H}^1 in terms of the mutually orthogonal, closed linear manifolds \mathcal{M} and \mathcal{N} .

THEOREM F.3 ([87] pages 189 and 247). *One of the three cases must occur:*

1. $\mathcal{E} = \emptyset$ and $\mathcal{M} = \{0\}$ has dimension zero; $\mathcal{N} = \mathcal{H}^1$ has countably infinite dimension. In this case, there exists an orthonormal set $\{\varphi_m\}$, $m = 1, 2, 3, \dots$, and mutually orthogonal, closed linear manifolds $\mathcal{N}(\varphi_m)$ which determine \mathcal{N} according to $\mathcal{N} = \bigoplus_{m=1}^{\infty} \mathcal{N}(\varphi_m)$.
2. \mathcal{E} contains an incomplete orthonormal set $\{\varphi_n\}$ so that both \mathcal{M} and \mathcal{N} are proper subsets of \mathcal{H}^1 , \mathcal{N} having countably infinite dimension and \mathcal{M} having finite or countably infinite dimension. In this case, there exists an orthonormal set $\{\varphi_m\}$ in \mathcal{N} . The closed linear manifolds $\mathcal{M}(\varphi_n)$ and $\mathcal{N}(\varphi_m)$ are mutually orthogonal and together determine \mathcal{H}^1 according to

$$\mathcal{M} = \bigoplus_{n=1}^{\infty} \mathcal{M}_n(\varphi_n), \quad \mathcal{N} = \bigoplus_{m=1}^{\infty} \mathcal{N}_m(\varphi_m), \quad \mathcal{H}^1 = \mathcal{M} \oplus \mathcal{N}$$

3. \mathcal{E} contains a complete orthonormal set $\{\varphi_n\}$; $\mathcal{M} = \mathcal{H}^1$ has countably infinite dimension; $\mathcal{N} = \{0\}$ has zero dimension. In this case, the closed linear manifolds $\mathcal{M}_n(\varphi_n)$ are mutually orthogonal and together determine \mathcal{M} according to $\mathcal{M} = \bigoplus_{n=1}^{\infty} \mathcal{M}_n(\varphi_n)$.

In each of the three cases, the closed linear manifolds \mathcal{M} and \mathcal{N} reduce A [87].

The following theorem characterizes eigenfunctions and eigenvalues in terms of $Q(\lambda)$.

THEOREM F.4. *The following are equivalent, necessary and sufficient conditions that an element $\varphi_n \in D(A)$ be an eigenfunction with eigenvalue $v_n = \imath\lambda_n$, $v_n \in \Sigma_{pp}$.*

1. $\|A\varphi_n - v_n\varphi_n\|^2 = 0$.
2. $\int_{-\infty}^{\infty} (\lambda - \lambda_n)^2 d\|Q(\lambda)\varphi_n\|_1^2 = 0$.
3. The function $\varrho_n(\lambda) = \|Q(\lambda)\varphi_n\|_1^2$ is constant on each of the intervals $-\infty < \lambda < \lambda_n$ and $\lambda_n < \lambda < \infty$.
4. $[Q(\lambda_n) - Q(\lambda_n^-)]\varphi_n = \varphi_n$, $\|\varphi_n\| = 1$.
5. $\|Q(\lambda)\varphi_n\|_1^2 = 0$, $Q(\lambda)\varphi_n = 0$ for $\lambda < \lambda_n$. While $\|Q(\lambda)\varphi_n - \varphi_n\|_1^2 = \|Q(\lambda)\varphi_n\|_1^2 - \|\varphi_n\|^2 = 0$, $Q(\lambda)\varphi_n = \varphi_n$ for $\lambda \geq \lambda_n$.

An immediate corollary of this theorem is the following. If φ_n is an eigenfunction associated with the eigenvalue $v_n = \imath\lambda_n$, then [87]

$$(F.33) \quad \|A\varphi_n\|_1^2 = \int_{-\infty}^{\infty} \lambda^2 d\|Q(\lambda)\varphi_n\|_1^2 = \lambda_n^2, \quad \langle A\varphi_n, h \rangle_1 = \int_{-\infty}^{\infty} \lambda d\langle Q(\lambda)\varphi_n, h \rangle_1 = \lambda_n \langle \varphi_n, h \rangle_1,$$

for all $h \in D(A)$. Moreover, a necessary and sufficient condition that $f \neq 0$ be an element of \mathcal{M} in cases (2) and (3) of Theorem F.3 is that

$$(F.34) \quad f = \sum_{n=1}^{\infty} a_n \varphi_n, \quad a_n = \langle f, \varphi_n \rangle_1, \quad \|f\|_1^2 = \sum_{n=1}^{\infty} |a_n|^2 \neq 0.$$

Furthermore, for such an element f we have

$$(F.35) \quad \|Q(\lambda)f\|_1^2 = \sum_{n: \lambda_n \leq \lambda} |a_n|^2, \quad A\varphi_n = \imath\lambda_n \varphi_n.$$

A characterization of continuous spectrum Σ_{cont} in terms of $Q(\lambda)$ and \mathcal{N} is the following. A necessary and sufficient condition that $f \neq 0$ be an element of \mathcal{N} is that $\|Q(\lambda)f\|_1^2$ be a continuous function of λ not identically zero. The following theorem is a refinement of cases (1) and (2) of Theorem F.3.

THEOREM F.5 ([87] page 250). *The orthonormal set $\{\varphi_m\}$ of Theorem F.3 can be replaced by an orthonormal set $\{\phi_m\}$ such that*

1. *The mutually orthogonal manifolds $\mathcal{N}(\phi_m)$ determine \mathcal{N} according to $\mathcal{N} = \oplus_{m=1}^{\infty} \mathcal{N}(\phi_m)$.*
2. *$\varrho_m(\lambda) = \|Q(\lambda)\phi_m\|_1^2$ is a continuous function of λ .*
3. *$\phi_1 \succ \phi_2 \succ \phi_3 \cdots$, where $\phi_k \succ \phi_{k+1}$ means*

$$(F.36) \quad \varrho_{k+1}(\lambda) = \int_{-\infty}^{\lambda} F(\psi) d\varrho_k(\psi), \quad \varrho_k(\lambda) = \|Q(\lambda)\phi_k\|_1^2, \quad F(\lambda) = \frac{d\varrho_{k+1}}{d\varrho_k},$$

where $F(\lambda)$ is real valued, non-negative, and uniquely determined.

The following theorem [87] provides an explicit representation for the standard decomposition of the Stieltjes measure $d\mu(\lambda)$ into its continuous and discrete components.

THEOREM F.6 ([87] page 189). *Let f be an arbitrary element of $D(A)$, and g and h be its (unique) projections on \mathcal{M} and \mathcal{N} , respectively, then the equation*

$$(F.37) \quad \|Q(\lambda)f\|_1^2 = \|Q(\lambda)g\|_1^2 + \|Q(\lambda)h\|_1^2, \quad d\|Q(\lambda)f\|_1^2 = d\|Q(\lambda)g\|_1^2 + d\|Q(\lambda)h\|_1^2$$

is valid and provides the standard resolution of the monotone function $\|Q(\lambda)f\|_1^2$ into its discontinuous and continuous monotone components, as well as the decomposition of the measure $d\|Q(\lambda)f\|_1^2$ into its discrete and continuous components. The function space \mathcal{N} can be further decomposed [79] $\mathcal{N} = \mathcal{N}_{\text{ac}} \otimes \mathcal{N}_{\text{sing}}$, with $h = h_{\text{ac}} + h_{\text{sing}}$, to provide the standard [33] decomposition of the continuous measure $d\|Q(\lambda)h\|_1^2$ into its components which are absolutely continuous and singular with respect to the Lebesgue measure, respectively,

$$(F.38) \quad d\|Q(\lambda)h\|_1^2 = d\|Q(\lambda)h_{\text{ac}}\|_1^2 + d\|Q(\lambda)h_{\text{sing}}\|_1^2.$$

However, the sets \mathcal{N}_{ac} and $\mathcal{N}_{\text{sing}}$ need not be disjoint [79].

We now use the mathematical framework summarized above to provide explicit formulas for the discrete component of the integral representations for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* , displayed in equation (2.14). For simplicity, we focus on the formulation of the effective parameter problem described by Corollary ??, as that of Theorem C.1 is analogous. Recall the cell problem of equations (2.12) and (F.21), written as

$$(F.39) \quad (\varepsilon + A)\chi_j = g_j, \quad g_j = (-\Delta)^{-1}u_j,$$

where A is defined in equation (2.11) and u_j , $j = 1, \dots, d$, is the j^{th} component of the velocity field \mathbf{u} . Since $\chi_j, g_j \in \mathcal{F} \subset \mathcal{H}^1$, by the formula $\mathcal{H}^1 = \mathcal{M} \oplus \mathcal{N}$ of Theorem F.3 and equation (F.34), they have the following representations

$$(F.40) \quad \chi_j = \sum_n \langle \varphi_n, \chi_j \rangle_1 \varphi_n + \chi_j^\perp, \quad g_j = \sum_n \langle \varphi_n, g_j \rangle_1 \varphi_n + g_j^\perp,$$

where $\varphi_n \in \mathcal{M}$ and $\chi_j^\perp, g_j^\perp \in \mathcal{N}$. Inserting (F.40) into the cell problem (F.39) and using $A\varphi_n = \imath\lambda_n\varphi_n$ yields

$$(F.41) \quad \sum_n [(\varepsilon + \imath\lambda_n) \langle \varphi_n, \chi_j \rangle_1 - \langle \varphi_n, g_j \rangle_1] \varphi_n + (\varepsilon + A)\chi_j^\perp - g_j^\perp = 0.$$

By the orthonormality of the set $\{\varphi_n\}$, the mutual orthogonality of the manifolds \mathcal{M} and \mathcal{N} , and since $\langle A\chi_j^\perp, \varphi_n \rangle_1 = -\langle \chi_j^\perp, A\varphi_n \rangle_1 = -\imath\lambda_n \langle \chi_j^\perp, \varphi_n \rangle_1 = 0$, taking the inner-product of both sides of (F.41) with φ_n yields

$$(F.42) \quad \langle \varphi_n, \chi_j \rangle_1 = \frac{\langle \varphi_n, g_j \rangle_1}{(\varepsilon + \imath\lambda_n)}, \quad 0 < \varepsilon < \infty.$$

Recall the representations $\mathbf{S}_{jk}^* = \varepsilon(\delta_{jk} + \langle \chi_j, \chi_k \rangle_1)$ and $\mathbf{A}_{jk}^* = \langle A\chi_j, \chi_k \rangle_1$, $j, k = 1, \dots, d$, displayed in equation (2.11). From equations (F.40) and (F.42), the orthonormality of the set $\{\varphi_n\}$, and the mutual

orthogonality of \mathcal{M} and \mathcal{N} , we have

$$(F.43) \quad \begin{aligned} \langle \chi_j, \chi_k \rangle_1 - \langle \chi_j^\perp, \chi_k^\perp \rangle_1 &= \sum_n \overline{\langle \varphi_n, \chi_j \rangle_1} \langle \varphi_n, \chi_k \rangle_1 = \sum_n \frac{\overline{\langle \varphi_n, g_j \rangle_1} \langle \varphi_n, g_k \rangle_1}{\varepsilon^2 + \lambda_n^2} \\ \langle A\chi_j, \chi_k \rangle_1 - \langle A\chi_j^\perp, \chi_k^\perp \rangle_1 &= \sum_n -i\lambda_n \overline{\langle \varphi_n, \chi_j \rangle_1} \langle \varphi_n, \chi_k \rangle_1 = \sum_n \frac{-i\lambda_n \overline{\langle \varphi_n, g_j \rangle_1} \langle \varphi_n, g_k \rangle_1}{\varepsilon^2 + \lambda_n^2}. \end{aligned}$$

The right hand sides of the formulas in equation (F.43) are Radon–Stieltjes integrals associated with a *discrete* measure. The terms $\langle \chi_j^\perp, \chi_k^\perp \rangle_1$ and $\langle A\chi_j^\perp, \chi_k^\perp \rangle_1$ also have Radon–Stieltjes integral representations involving the *continuous* measure $d\langle Q(\lambda)g_j^\perp, g_k^\perp \rangle_1$, and provides the standard decomposition of the *spectral measure* into its discrete and continuous components, in the general setting [87].

A direct correspondence can be made between the integrals in equations (F.43) and (2.14) with use of Dirac’s bra-ket notation as follows. Writing $\mu_{jk}(\lambda) = \langle Q(\lambda)g_j, g_k \rangle_1 = \langle g_j, Q(\lambda)g_k \rangle_1 = \langle g_j | Q(\lambda) | g_k \rangle$ and recalling the property $\overline{\langle \varphi_n, g_j \rangle_1} = \langle g_j, \varphi_n \rangle_1$ and that g_j is real-valued, suggests the notation

$$(F.44) \quad \overline{\langle \varphi_n, g_j \rangle_1} \langle \varphi_n, g_k \rangle_1 = \langle g_j | \langle \varphi_n | \langle \varphi_n | g_j \rangle = \langle g_j | Q_n | g_k \rangle,$$

where $Q_n = |\varphi_n\rangle\langle\varphi_n|$, $n = 1, 2, 3, \dots$, are mutually orthogonal projection operators satisfying $Q_n Q_m = Q_n \delta_{nm}$, as $\langle \varphi_n, \varphi_m \rangle_1 = \langle \varphi_n | \varphi_m \rangle = \delta_{nm}$. With this notation, the spectral measure $d\mu_{jk}(\lambda)$ and projection valued operator $Q(\lambda)$ are given by

$$(F.45) \quad d\mu_{jk}(\lambda) = \langle g_j | Q(\lambda) | g_k \rangle \delta_{\lambda_n}(d\lambda), \quad Q(\lambda) = \sum_{n: \lambda_n \leq \lambda} Q_n, \quad Q_n = |\varphi_n\rangle\langle\varphi_n|, \quad \lambda \in \Sigma_{pp}(A),$$

where $\delta_{\lambda_n}(d\lambda)$ is the delta measure concentrated at λ_n . Moreover, exactly as in equations (??) and (??), we may use the fact that the function g_j and molecular diffusivity ε are real-valued, to re-express the integrals in (F.43), involving the *complex measure* $d\mu_{jk}(\lambda)$, in terms of the *signed measures* $d\text{Re } \mu_{jk}(\lambda) := (d\mu_{jk}(\lambda) + d\mu_{kj}(\lambda))/2$ and $d\text{Im } \mu_{jk}(\lambda) := (d\mu_{jk}(\lambda) - d\mu_{kj}(\lambda))/(2i)$, where

$$(F.46) \quad \begin{aligned} d\text{Re } \mu_{jk}(\lambda) &= \text{Re} \langle g_j | Q(\lambda) | g_k \rangle \delta_{\lambda_n}(d\lambda), & \text{Re} \langle g_j | Q(\lambda) | g_k \rangle &= \sum_{n: \lambda_n \leq \lambda} \text{Re} [\overline{\langle \varphi_n, g_j \rangle_1} \langle \varphi_n, g_k \rangle_1] \\ d\text{Im } \mu_{jk}(\lambda) &= \text{Im} \langle g_j | Q(\lambda) | g_k \rangle \delta_{\lambda_n}(d\lambda), & \text{Im} \langle g_j | Q(\lambda) | g_k \rangle &= \sum_{n: \lambda_n \leq \lambda} \text{Im} [\overline{\langle \varphi_n, g_j \rangle_1} \langle \varphi_n, g_k \rangle_1]. \end{aligned}$$

A useful property of the inner-product $\langle \varphi_n, g_k \rangle_1$ and the form of $g_j = (-\Delta)^{-1}u_j$ is that $\langle \varphi_n, g_j \rangle_1 = \langle \varphi_n, u_j \rangle_2$. More specifically, since $u_j(t, \cdot) \in \mathcal{H}^1(\mathcal{V}) \subset L^2(\mathcal{V})$ we have [85]

$$(F.47) \quad \langle \varphi_n, g_j \rangle_1 = \langle \nabla \varphi_n \cdot \nabla (-\Delta)^{-1}u_j \rangle = \langle \varphi_n, (-\Delta)(-\Delta)^{-1}u_j \rangle_2 = \langle \varphi_n, u_j \rangle_2,$$

where $\langle \cdot, \cdot \rangle_2$ denotes the $L^2(\mathcal{T} \times \mathcal{V})$ inner-product. This property will be used in Section 3 to calculate S_{jk}^* and A_{jk}^* for a large class of velocity fields.

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