

Spectral analysis and computation of effective diffusivities in space-time periodic incompressible flows

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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 computations in a low dimensional subspace capture the phenomenon of residual diffusion related to Lagrangian chaos of the flow, which is reflected in the spectral measure by a concentration of mass near the spectral origin.

KEYWORDS AND PHRASES: advective diffusion, homogenization, effective diffusivity, spectral measure, integral formula, Fourier method, generalized eigenvalue computation, residual diffusion.

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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 [88] with an effective diffusivity tensor \mathbf{D}^* . Describing the associated transport properties is a challenging problem with a broad range of scientific and engineering applications, such as stellar convection [45, 76, 20, 21, 19], turbulent combustion [3, 16, 87], and solute transport in porous media [13, 14, 92, 39, 46, 49, 47]. 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 [25, 38], turbulence plays a key role in transporting mass, heat, momentum, energy, and salt in geophysical flows [63]. Turbulence enhances the dispersion of atmospheric gases [27] such as ozone [41, 73, 74, 75] and pollutants [24, 10, 80], as well as atmosphere-ocean transfers of carbon dioxide and other climatically important trace gas fluxes [94, 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 [93, 48, 17]. Chaotic motion of time-dependent fluid velocity fields cause instabilities in large scale ocean currents, generating geostrophic eddies [31] which dominate the kinetic energy of the ocean [32]. Geostrophic eddies greatly enhance [31] 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 [83]. 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 [22]. In sea ice, which couples the atmosphere to the polar oceans [90], the transport of vast ice floes can also be enhanced by eddy fluxes [91, 51].

It has been noted in various geophysical contexts [74, 75] that eddy-induced, skew-diffusive tracer fluxes, directed normal to the tracer gradient [60], are generally equivalent to antisymmetric components in the effective diffusivity tensor \mathbf{D}^* , while the symmetric part of \mathbf{D}^* represents irreversible diffusive effects [77, 81, 37] directed down the tracer gradient. The mixing of eddy fluxes is typically non-divergent and unable to affect the evolution of the mean flow [60], and do not alter the tracer moments [37]. In this sense, the mixing is non-dissipative, reversible, and sometimes referred to as stirring [26, 37]. 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 [70]. This suggests

that the effective diffusivity tensor D^* should be spatially and possibly also temporally inhomogeneous [70].

Due to the computational intensity of detailed climate models [38, 90, 66], 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 [50], atmospheric boundary layer turbulence [18], atmosphere-surface exchange over the sea [28] and sea ice [82, 1, 2, 89], and eddies in the ocean [56, 35]. 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 [67, 57, 8, 15, 29, 30, 55, 70, 72, 23, 40, 42, 53, 54]. Motivated by [68], it was shown [57] 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 [57]. 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 [57].

The incompressibility condition of the time-independent fluid velocity field was used [4, 5] to transform the cell problem in [57] into the quasi-static limit of Maxwell’s equations [44, 36], which describe the transport properties of an electromagnetic wave in a composite material [62]. The analytic continuation method for representing transport in composites [36] provides Stieltjes integral representations for the bulk transport coefficients of composite media, such as electrical conductivity and permittivity, magnetic permeability, and thermal conductivity [62]. This method is based on the spectral theorem [86, 78] and a resolvent formula for, say, the electric field, involving a random self-adjoint operator [36, 65] or matrix [64]. Based on [36], 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, 29, 30].

The mathematical framework developed in [57] was adapted [70, 58, 53] 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 [70] 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 [70]. This is consistent with what has been observed in geophysical flows in the climate system, as discussed above. In [58], this result was extended to weakly compressible, anelastic fluid velocity fields.

Based on [13], the cell problem discussed in [70] was transformed into a resolvent formula involving a self-adjoint operator, acting on the Sobolev space [59, 33] 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 [13], hence *bounded* [84]. 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 [70] 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 [70] 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 the following space-time periodic flow in two spatial dimensions, with $\mathbf{x} = (x, y)$,

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

The steady part $(\cos y, \cos x)$ of the flow is subject to a time-periodic perturbation that causes transition to Lagrangian chaos [15, 95]. In the advection dominated regime, we shall compare our computations of the effective diffusivity for the steady $\theta = 0$ and dynamic $\theta = 1$ settings.

The rest of the paper is organized as follows. In Section 2 the theory of homogenization for the advection-diffusion equation for space-time periodic flows is reviewed. Novel Stieltjes integral representations for the effective diffusivity tensor are also obtained for a large class of fluid velocity fields, involving a spectral measure of an *unbounded* self-adjoint operator. In Section 3 we use Fourier methods to transform the eigenvalue problem for the operator into an infinite set of algebraic equations. This provides a rigorous mathematical foundation for the computation of effective diffusivities for such flows. This framework is employed in Section 4 to compute the discrete component of the spectral measure associated with the fluid velocity field in (1) for time-independent flow $\theta = 0$ and time-dependent flow $\theta = 1$. Our computations highlight that the behavior of the measure near the spectral origin governs the behavior of the effective diffusivity in the advection dominated regime of small molecular diffusion. In particular, we demonstrate that for $\theta = 0$ there is a *spectral gap* in the measure near a limit point at the

spectral origin, giving rise to the known vanishing asymptotic behavior of 2D cell flows [29]. However in the time dependent setting, a strong concentration of measure mass near the spectral origin gives rise to the phenomenon of residual diffusivity in the limit of vanishing molecular diffusion.

The proofs of the integral representation formulas for the effective diffusivity, over both vector and scalar fields, as well as background material, are in the appendices. The spectral theory of unbounded self-adjoint operators in Hilbert space is reviewed in Sections A and B. Two mathematical formulations of the effective parameter problem for advection enhanced diffusion are presented in Section C, leading to novel integral representations for the symmetric and antisymmetric components of the effective diffusivity tensor. In Section D we use powerful methods of functional analysis to prove that the two approaches are equivalent, which follows from a one-to-one isometry between the associated Hilbert spaces. In Section D.1 we derive an explicit formula for the discrete component of the spectral measure, which is employed in our numerical computations.

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

$$(2) \quad \partial_t \phi(t, \mathbf{x}) = \mathbf{u}(t, \mathbf{x}) \cdot \nabla \phi(t, \mathbf{x}) + \varepsilon \Delta \phi(t, \mathbf{x}), \quad \phi(0, \mathbf{x}) = \phi_0(\mathbf{x}),$$

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), the molecular diffusion constant $\varepsilon > 0$, 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) 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) 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 [58, 53]. Here, we focus on the long time, large scale transport characteristics of equation (2) 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.,

$$(3) \quad \mathbf{u}(t+T, \mathbf{x}) = \mathbf{u}(t, \mathbf{x}), \quad \mathbf{u}(t, \mathbf{x} + \ell \mathbf{e}_j) = \mathbf{u}(t, \mathbf{x}), \quad j = 1, \dots, d,$$

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 [88] with an effective diffusivity tensor \mathbf{D}^* . In recent decades, methods of homogenization theory [57, 29, 53] have been used to provide an explicit representation for \mathbf{D}^* . In particular, these methods have demonstrated that the averaged or *homogenized* behavior of the advection-diffusion equation in (2), 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 \mathbf{D}^* [53]

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

Equation (4) follows from the assumption that the initial tracer density ϕ_0 varies slowly relative to the variations of the fluid velocity field \mathbf{u} [57, 30, 53]. This information is incorporated into equation (2) by introducing a small dimensionless parameter $\delta \ll 1$ and writing [57, 30, 53]

$$(5) \quad \phi(0, \mathbf{x}) = \phi_0(\delta \mathbf{x}).$$

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

$$(6) \quad \boldsymbol{\xi} = \mathbf{x}/\delta, \quad \tau = t/\delta^\gamma, \quad \gamma = 2.$$

The rescaled form of equation (2) is given by [53]

$$(7) \quad \partial_t \phi^\delta(t, \mathbf{x}) = \delta^{-1} \mathbf{u}(t/\delta^2, \mathbf{x}/\delta) \cdot \nabla \phi^\delta(t, \mathbf{x}) + \varepsilon \Delta \phi^\delta(t, \mathbf{x}), \quad \phi(0, \mathbf{x}) = \phi_0(\mathbf{x}),$$

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 [53]

$$(8) \quad \lim_{\delta \rightarrow 0} \sup_{0 \leq t \leq t_0} \sup_{\mathbf{x} \in \mathbb{R}^d} |\phi^\delta(t, \mathbf{x}) - \bar{\phi}(t, \mathbf{x})| = 0,$$

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* [15, 53],

$$(9) \quad \partial_\tau \chi_j(\tau, \boldsymbol{\xi}) - \varepsilon \Delta_\xi \chi_j(\tau, \boldsymbol{\xi}) - \mathbf{u}(\tau, \boldsymbol{\xi}) \cdot \nabla_\xi \chi_j(\tau, \boldsymbol{\xi}) = u_j(\tau, \boldsymbol{\xi}),$$

where the subscript ξ in Δ_ξ and ∇_ξ indicates that differentiation is with respect to the fast variable $\boldsymbol{\xi}$ defined in equation (6). Specifically, the components \mathbf{D}_{jk}^* , $j, k = 1, \dots, d$, of the matrix \mathbf{D}^* are given by [57, 29, 53]

$$(10) \quad \mathbf{D}_{jk}^* = \varepsilon \delta_{jk} + \langle u_j \chi_k \rangle,$$

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 (10) is with respect to the fast variables defined in equation (6). 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 (9) with $\partial_\tau \chi_j \equiv 0$, and $\langle \cdot \rangle$ in (10) denotes spatial averaging over \mathcal{V} [29, 53]. Since the remainder of the analysis involves only the fast variables, for notational simplicity, we will drop the subscripts ξ displayed in equation (9).

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

$$(11) \quad \mathbf{D}^* = \mathbf{S}^* + \mathbf{A}^*, \quad \mathbf{S}^* = \frac{1}{2} (\mathbf{D}^* + [\mathbf{D}^*]^T), \quad \mathbf{A}^* = \frac{1}{2} (\mathbf{D}^* - [\mathbf{D}^*]^T),$$

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 (11). In Section C.1 we show that they have the following functional representations [70]

$$(12) \quad \mathbf{S}_{jk}^* = \varepsilon (\delta_{jk} + \langle \chi_j, \chi_k \rangle_1), \quad \mathbf{A}_{jk}^* = \langle A \chi_j, \chi_k \rangle_1, \quad A = (-\Delta)^{-1} (\partial_\tau - \mathbf{u} \cdot \nabla),$$

where $\langle f, h \rangle_1 = \langle \nabla f \cdot \nabla h \rangle$ is a Sobelov-type *sesquilinear* inner-product [59] and the operator $(-\Delta)^{-1}$ is based on convolution with respect to the Green's function for the Laplacian Δ [84]. 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 (9) yields the following resolvent formula for χ_j

$$(13) \quad \chi_j = (\varepsilon + A)^{-1}g_j, \quad g_j = (-\Delta)^{-1}u_j.$$

From equations (12) and (13) we have the following functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* involving the antisymmetric operator A

$$(14) \quad \mathbf{S}_{jk}^* = \varepsilon (\delta_{jk} + \langle (\varepsilon + A)^{-1}g_j, (\varepsilon + A)^{-1}g_k \rangle_1), \quad \mathbf{A}_{jk}^* = \langle A(\varepsilon + A)^{-1}g_j, (\varepsilon + A)^{-1}g_k \rangle_1.$$

Since A is a skew-symmetric operator, it can be written as $A = \imath M$ 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 [86] $\lim_{\lambda \rightarrow \inf \Sigma} Q(\lambda) = 0$ and $\lim_{\lambda \rightarrow \sup \Sigma} Q(\lambda) = I$ [86], 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 (13). 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 (36). Then, given certain regularity conditions on the components u_j of the fluid velocity field \mathbf{u} , the functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* in (14) have the following Radon–Stieltjes integral representations, for all $0 < \varepsilon < \infty$ (see Section C.1 for details)

$$(15) \quad \mathbf{S}_{jk}^* = \varepsilon \left(\delta_{jk} + \int_{-\infty}^{\infty} \frac{d\text{Re } \mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2} \right), \quad \mathbf{A}_{jk}^* = - \int_{-\infty}^{\infty} \frac{\lambda d\text{Im } \mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2}.$$

The periodic homogenization theorem summarized by equations (3)–(10), as well as its many variations [8, 67, 12, 14, 57, 5, 70, 71, 72, 58, 53], depend on the detailed nature of the fluid velocity field \mathbf{u} . They also depend on the temporal scaling used [14, 70, 53], i.e., what value of γ is used in equation (6). However, the mathematical structure of the cell problem in (9)

and the functional form of \mathbf{D}^* displayed in equation (10) 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 the Stieltjes integral representations for effective diffusivity tensor \mathbf{D}^* displayed in (15), for space-time periodic \mathbf{u} . Due to the time-dependence of the fluid velocity field, one must employ the spectral theory of *unbounded* self-adjoint operators, which is much more subtle and challenging than that of bounded operators. We will demonstrate that this mathematical framework depends only on the structure of the cell problem in (9) and the presence of an inner-product in the functional form of \mathbf{D}^* in (10). In particular, the theoretical development is insensitive to the detailed nature of \mathbf{u} and depends only on its boundedness properties (See Corollary 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 \mathbf{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 (8) holds and the effective diffusivity tensor \mathbf{D}^* defined in (10) is constant [53]. Consequently, only the symmetric part of \mathbf{D}^* plays a role in the effective transport equation displayed in (4). Now consider a more general fluid velocity field

$$(16) \quad \mathbf{u}(t, \mathbf{x}) = \delta^\alpha \mathbf{u}_0(\delta^\gamma t, \delta \mathbf{x}) + \mathbf{u}_1(t, \mathbf{x}), \quad \alpha = 1, \quad \gamma = 2,$$

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 [53]. 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 (4) is replaced by [53]

$$(17) \quad \partial_t \bar{\phi}(t, \mathbf{x}) = \mathbf{u}_0(t, \mathbf{x}) \cdot \nabla \bar{\phi}(t, \mathbf{x}) + \nabla \cdot [\mathbf{D}^* \nabla \bar{\phi}(t, \mathbf{x})], \quad \bar{\phi}(0, \mathbf{x}) = \phi_0(\mathbf{x}),$$

which includes an advective enhancement in transport by the large-scale mean flow \mathbf{u}_0 [53]. In this case, the effective diffusivity tensor \mathbf{D}^* is completely independent of the mean flow \mathbf{u}_0 , and is determined by the same formula in equation (10) and the same cell problem in (9) with $\mathbf{u} \rightarrow \mathbf{u}_1$ [53]. Consequently, \mathbf{D}^* is again constant and only the symmetric part of \mathbf{D}^* plays a role in the effective transport equation displayed in (17).

This problem was studied in [70] for scalings in (16) 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 (17) [70]. 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 (10) and the structure of the cell problem is analogous to equation (9). There are three distinct behaviors that arise as the values of α and γ vary, and the function χ_j in (9) can be time-dependent or time-independent ($\partial_\tau \chi_j \equiv 0$) [70].

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* [70]. 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 [70]. 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 framework that leads to the Stieltjes integral representations in (15), 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. 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 D 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.

3. Fourier methods

In this section we discuss how Fourier methods can be employed to convert the eigenvalue problem $A\varphi_l = \imath\lambda_l\varphi_l$, $\lambda_l \in \mathbb{R}$, $l \in \mathbb{N}$, into an infinite set of algebraic equations involving the Fourier coefficients of the eigenfunction φ_l . This will be used in Section 4 to compute the discrete component of the spectral measure μ_{jk} underlying the integral representations for the effective diffusivity tensor \mathbf{D}^* displayed in equations (15) and (85). For notational simplicity, we set $\mathbf{u} \rightarrow -\mathbf{u}$ and $(\tau, \boldsymbol{\xi}) \rightarrow (t, \mathbf{x})$ and write the operator A in (12) as $A = (-\Delta)^{-1}(\partial_t + \mathbf{u} \cdot \nabla)$. We will focus on the fluid velocity field \mathbf{u} in equation (1), although the methods discussed here extend to a large class of fluid velocity fields, namely, those expressible as a finite sum of Fourier modes.

In Section C.1 we showed that $M = -\imath A$ is a self-adjoint operator on an appropriate, densely defined subset of a Hilbert space $\mathcal{H} \subset L^2(\mathcal{T} \times \mathcal{V})$ given in equation (48). Since the space-time periodic velocity field \mathbf{u} in (1) is mean-zero, we require that the elements of \mathcal{H} are also mean-zero, i.e., $f \in \mathcal{H}$ implies that $\langle f \rangle = 0$. In Section D.1 we discuss how a decomposition of the Hilbert space \mathcal{H} provides a natural decomposition of the spectral measure μ_{jk} into its discrete and continuous components, as displayed in equation (80). Here, we demonstrate how this mathematical framework can be used to compute the discrete component of μ_{jk} , hence the discrete component of the Stieltjes integral representation for the effective diffusivity tensor \mathbf{D}^* displayed in equation (85).

Toward this goal, rewrite the eigenvalue problem $A\varphi_l = \imath\lambda_n\varphi_l$ as

$$(18) \quad (\partial_t + \mathbf{u} \cdot \nabla)\varphi_l = -\imath\lambda_n\Delta\varphi_l.$$

For spatial dimension $d = 2$, the set of functions $\{\exp[\imath(\ell t + m x + n y)] \mid \ell, m, n \in \mathbb{Z}\}$ are complete in $L^2(\mathcal{T} \times \mathcal{V})$, hence the Hilbert space \mathcal{H} . Consequently, the eigenfunction $\varphi_l \in \mathcal{H}$ can be represented as

$$(19) \quad \varphi_l(t, \mathbf{x}) = \sum_{\ell, m, n} a_{\ell, m, n}^l e^{\imath(\ell t + m x + n y)}, \quad a_{\ell, m, n}^l = \left\langle \varphi_l, e^{\imath(\ell t + m x + n y)} \right\rangle, \quad \ell, m, n \in \mathbb{Z},$$

where we have denoted $\mathbf{x} = (x, y)$ and $\langle \cdot, \cdot \rangle$ is the $L^2(\mathcal{T} \times \mathcal{V})$ -inner-product. Write the fluid velocity field in (1) as $\mathbf{u}(t, \mathbf{x}) = \mathbf{u}_1(\mathbf{x}) + \theta \cos t \mathbf{u}_2(\mathbf{x})$, where

$\mathbf{u}_1 = (\cos y, \cos x)$ and $\mathbf{u}_2 = (\sin y, \sin x)$, and write

$$(20) \quad \cos t \sin y = \frac{1}{4i}(e^{it} + e^{-it})(e^{iy} - e^{-iy}) = \frac{1}{4i}(e^{i(t+y)} - e^{i(t-y)} + e^{i(-t+y)} - e^{i(-t-y)})$$

Consequently, substituting the formula in (19) for φ_l into equation (18) yields

$$(21) \quad 0 = \sum_{\ell, m, n} e^{i(\ell t + m x + n y)} \left[i\ell a_{\ell, m, n}^l - i\lambda_l(m^2 + n^2)a_{\ell, m, n}^l \right. \\ \left. + im((a_{\ell, m, n-1}^l + a_{\ell, m, n+1}^l)/2 + \theta(a_{\ell-1, m, n-1}^l - a_{\ell-1, m, n+1}^l + a_{\ell+1, m, n-1}^l - a_{\ell+1, m, n+1}^l)/(4i)) \right. \\ \left. + in((a_{\ell, m-1, n}^l + a_{\ell, m+1, n}^l)/2 + \theta(a_{\ell-1, m-1, n}^l - a_{\ell-1, m+1, n}^l + a_{\ell+1, m-1, n}^l - a_{\ell+1, m+1, n}^l)/(4i)) \right].$$

Since the orthonormal set $\{e^{i(\ell t + m x + n y)}\}$ is complete, $\sum_{\ell, m, n} e^{i(\ell t + m x + n y)} c_{\ell, m, n} = 0$ only if $c_{\ell, m, n} = 0$ for all $\ell, m, n \in \mathbb{Z}$. Consequently, equation (21) yields the following infinite set of algebraic equations for the Fourier coefficients $a_{\ell, m, n}^l$ of the eigenfunction φ_l

$$(22) \quad i\ell a_{\ell, m, n}^l + \frac{i}{2}[m(a_{\ell, m, n-1}^l + a_{\ell, m, n+1}^l) + n(a_{\ell, m-1, n}^l + a_{\ell, m+1, n}^l)] \\ + \frac{\theta}{4}[m(a_{\ell-1, m, n-1}^l - a_{\ell-1, m, n+1}^l) + n(a_{\ell-1, m-1, n}^l - a_{\ell-1, m+1, n}^l) \\ + m(a_{\ell+1, m, n-1}^l - a_{\ell+1, m, n+1}^l) + n(a_{\ell+1, m-1, n}^l - a_{\ell+1, m+1, n}^l)] \\ = i\lambda_l(m^2 + n^2)a_{\ell, m, n}^l, \quad \ell, m, n \in \mathbb{Z},$$

The solution of equation (22) determines both the eigenvalues λ_l and the Fourier coefficients $a_{\ell, m, n}^l$ of the eigenfunction φ_l . Notice that for $m = n = 0$, equation (22) implies that $i\ell a_{\ell, 0, 0}^l = 0$ for all $\ell \in \mathbb{Z}$. This is consistent. In fact, the requirement that φ_l is mean-zero $\langle \varphi_l \rangle = 0$ in both space and time implies that $a_{\ell, 0, 0}^l = 0$ for all $\ell \in \mathbb{Z}$ and $a_{0, m, n}^l = 0$ for all $m, n \in \mathbb{Z}$. This will be used in Section 4 to compute the discrete component of the spectral measure μ_{jk} .

Towards this goal, we now determine the spectral weights $\langle g_j, \varphi_l \rangle_1$ of the measure μ_{jk} displayed in (85) in terms of the Fourier coefficients $a_{\ell, m, n}^l$ of φ_l . Recall that $\mathbf{u}(t, \mathbf{x}) = \mathbf{u}_1(\mathbf{x}) + \theta \cos t \mathbf{u}_2(\mathbf{x})$ with $\mathbf{u}_1 = (\cos y, \cos x)$ and

$\mathbf{u}_2 = (\sin y, \sin x)$ and write

(23)

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

and $u_2(t, x, y) = u_1(t, y, x)$. This equation, the formula $\langle g_j, \varphi_l \rangle_1 = \langle u_j, \varphi_l \rangle_2$ in equation (86), the Fourier expansion of φ_l in (19), and the orthogonality of the set $\{e^{i(\ell t + mx + ny)}\}$, imply that

(24)

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

with $\langle g_1, \varphi_l \rangle_1 = \overline{\langle \varphi_l, g_1 \rangle_1}$.

When $\theta = 0$ in the velocity field of equation (1) so that $\mathbf{u} = \mathbf{u}(\mathbf{x})$ is time-independent, the operator A no longer involves the time derivative and the associated eigenfunction $\varphi_l = \varphi_l(\mathbf{x})$ is time-independent as well. In this case, the system of equations in (22) reduces to

(25)

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

while equation (24) for the reduces to

$$(26) \quad \langle \varphi_l, g_1 \rangle_1 = \frac{1}{2} (a_{0,1}^l + a_{0,-1}^l), \quad \langle \varphi_l, g_2 \rangle_1 = \frac{1}{2} (a_{1,0}^l + a_{-1,0}^l).$$

4. Numerical Results

In Section 3, we used Fourier methods to transform the eigenvalue problem $A\varphi_l = \iota\lambda_l\varphi_l$ for the operator A in (12), involving the fluid velocity field in (1), into an infinite system of algebraic equations for the Fourier coefficients of the eigenfunctions φ_l . In this section, we truncate the infinite system, convert it to a generalized eigenvalue problem, and numerically compute the discrete component of the spectral measure underlying the integral representations for the symmetric \mathbf{S}^* and anti-symmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* , displayed in equations (15) and (85).

By restricting the indices, $-M \leq \ell, m, n \leq M$, and imposing the boundary conditions

$$(27) \quad a_{\ell, m, n}^l = 0 \quad \text{if} \quad \max(|\ell|, |m|, |n|) > M,$$

the infinite systems of equations in (22) and (25) become finite sets of equations. Consider the fluid velocity field in (1) with parameter $\theta \in [0, 1]$. In the dynamic ($\theta > 0$) and steady ($\theta = 0$) cases, the bijective mappings $\Theta_d(\ell, m, n)$ and $\Theta_s(m, n)$ defined by

$$(28) \quad \begin{aligned} \Theta_d(\ell, m, n) &= (M + m + 1) + (M + n)(2M + 1) + (M + \ell)(2M + 1)^2, \\ \Theta_s(m, n) &= (M + m + 1) + (M + n)(2M + 1), \end{aligned}$$

map the corresponding finite set of equations to matrix equations. In particular, they become generalized eigenvalue problems

$$(29) \quad \mathbf{B}\mathbf{a}_l = \lambda_l \mathbf{C}\mathbf{a}_l.$$

Here \mathbf{B} is a symmetric matrix and \mathbf{C} is a diagonal matrix of size $(2M + 1)^3 \times (2M + 1)^3$ for the dynamic case and of size $(2M + 1)^2 \times (2M + 1)^2$ for the steady case. More specifically, \mathbf{B} is Hermitian in the dynamic case and is real-symmetric in the steady case, while the matrix \mathbf{C} is real-symmetric and diagonal in both cases. Since \mathbf{B} and \mathbf{C} are symmetric matrices, the generalized eigenvalues λ_l are real-valued and the eigen-vectors \mathbf{a}_l – consisting of the Fourier coefficients for φ_l – satisfy the orthogonality condition [69]

$$(30) \quad \mathbf{a}_j^\dagger \mathbf{C} \mathbf{a}_k = \delta_{jk}.$$

The matrix \mathbf{C} is positive semidefinite and diagonal. However, in the steady case, in both of the matrices \mathbf{B} and \mathbf{C} , the row and column associated with the Fourier coefficient $a_{0,0}^l$ is all zeros, as can be seen from equation (25). Since the eigenfunction φ_l is mean-zero, we have that $a_{0,0}^l = 0$. Therefore, we simply remove this row and column in both \mathbf{B} and \mathbf{C} so that \mathbf{C} becomes strictly positive definite.

In the dynamic case, the entries of the matrix \mathbf{C} do not depend on ℓ . Consequently, we have that $\mathbf{C} = \text{diag}(\mathbf{C}_s, \dots, \mathbf{C}_s)$, where we have denoted by \mathbf{C}_s the matrix \mathbf{C} in the steady case. Therefore, there are $2M + 1$ diagonal entries in \mathbf{C} with the value zero, corresponding to $m = n = 0$. The entries of the corresponding rows and columns of the matrix \mathbf{B} are all zero except for

the diagonal entry, which has the value ℓ , as can be seen from equation (22). This implies that $\ell a_{\ell,0,0}^l = 0$ for all $-M \leq \ell \leq M$. Since the eigenfunction φ_l is mean-zero in time *and* space, we have that $a_{\ell,0,0}^l = 0$ for all $-M \leq \ell \leq M$, which is consistent with the above observation. We therefore simply remove the corresponding rows and columns in both \mathbf{B} and \mathbf{C} so that \mathbf{C} becomes strictly positive definite. This method of removing the null space common to both \mathbf{B} and \mathbf{C} is called *deflation* [69].

Now that the matrix \mathbf{C} is strictly positive definite and diagonal, the matrix \mathbf{C}^q is well defined for all $q \in \mathbb{R}$, with entries $(\mathbf{C}^q)_{ij} = \mathbf{C}_{ii}^q \delta_{ij}$, where \mathbf{C}_{ii}^q is the i th diagonal of the matrix \mathbf{C} raised to the power q , and $\mathbf{C}^q \mathbf{C}^{-q} = \mathbf{I}$. Consequently, the generalized eigenvalue problem in equation (29) can be written as the following standard eigenvalue problem

$$(31) \quad \mathbf{C}^{-1/2} \mathbf{B} \mathbf{C}^{-1/2} \mathbf{v}_l = \lambda_l \mathbf{v}_l, \quad \mathbf{v}_l = \mathbf{C}^{1/2} \mathbf{a}_l.$$

Since \mathbf{B} is a symmetric matrix and \mathbf{C} is diagonal, the matrix $\mathbf{C}^{-1/2} \mathbf{B} \mathbf{C}^{-1/2}$ is also symmetric with real-valued eigenvalues and orthonormal eigenvectors. From the orthogonality relation $\mathbf{v}_j^\dagger \mathbf{v}_k = \delta_{jk}$ we recover equation (30) via $\mathbf{v}_l = \mathbf{C}^{1/2} \mathbf{a}_l$ in (31).

In summary, our numerical method is the following. Create the matrices \mathbf{B} and \mathbf{C} according to equation (22) or (25) and the corresponding bijective mapping in (28). Remove the rows and columns of the matrices \mathbf{B} and \mathbf{C} corresponding to $\mathbf{C}_{ii} = 0$. Compute the eigenvalues λ_l and eigenvectors \mathbf{v}_l of the symmetric matrix $\mathbf{C}^{-1/2} \mathbf{B} \mathbf{C}^{-1/2}$. The computed Fourier coefficients of the eigenfunction φ_l are given by $\mathbf{a}_l = \mathbf{C}^{-1/2} \mathbf{v}_l$. The eigenvalues associated with the discrete component of the spectral measure displayed in equation (85) are given by λ_l , while the spectral measure weights $\langle g_1, \varphi_l \rangle_1$ and $\langle g_2, \varphi_l \rangle_1$ in (85) are determined by the vector \mathbf{a}_l via equation (24) or (26).

In our computations, we used for the steady case $M = 150$, yielding matrices of size $(2M + 1)^2 - 1 = 90,600$, while in the dynamic case we used $M = 20$, yielding matrices of size $(2M + 1)^3 - (2M + 1) = 68,880$. The eigenvalues and eigenvectors of the symmetric matrix $\mathbf{C}^{-1/2} \mathbf{B} \mathbf{C}^{-1/2}$ were computed using the Matlab function `eig()`. The stability of the computations are measured in terms of the condition numbers \mathcal{K}_l of the eigenvalues λ_l , which are the reciprocals of the cosines of the angles between the left and right eigenvectors. Eigenvalue condition numbers close to 1 indicate a stable computation. Our eigenvalue computations are extremely stable with $\max_l |1 - \mathcal{K}_l| \sim 10^{-14}$, which were computed using the Matlab function `condeig()`.

Displayed in Fig. 1 are our computations of the discrete component of the spectral measure $d\mu_{11}(\lambda) = \sum_l m_{11}(l)\delta_{\lambda_l}(d\lambda)$ associated with the fluid velocity field \mathbf{u} displayed in equation (1), for (a) the steady ($\theta = 0$) and (b) the dynamic ($\theta = 1$) settings. Here, the spectral weights $m_{11}(l) = |\langle g_1, \varphi_l \rangle_1|^2$ are determined by equations (26) and (24), respectively. Consistent with the symmetries of the flows [15], we have $\mu_{11} = \mu_{22}$, while $\text{Re } \mu_{12} = 0$ and $\text{Im } \mu_{12} = 0$, up to numerical accuracy and finite size effects. For the 2D steady cell flow in (1) with $\theta = 0$, it is known [29] that $S_{11}^* \sim \varepsilon^{1/2}$ for $\varepsilon \ll 1$. Our computation of S_{11}^* displayed in Fig. 1(c) is in excellent agreement with this result, with a computed critical exponent of ≈ 0.52 having an error of only 4% relative to its true value 0.5. In this steady setting, the underlying operator $(-\Delta)^{-1}[\mathbf{u}_1 \cdot \nabla]$ is compact [13] and therefore has bounded, discrete spectrum away from the spectral origin, with a limit point at $\lambda = 0$ [84]. The limit point behavior of the measure μ_{11} can be seen in the rightmost panel of Fig. 1(a). The decay of S_{11}^* for vanishing ε is due to the magnitude of the measure masses $m_{11}(l) \lesssim 10^{-30}$ for $|\lambda_l| \ll 1$, with a *spectral gap* near the limit point. The rigorous result [29] $S_{11}^* \sim \varepsilon^{1/2}$ as $\varepsilon \rightarrow 0$ demonstrates that the spectral measure μ_{11} of the operator $(-\Delta)^{-1}[\mathbf{u}_1 \cdot \nabla]$ is *continuous* at $\lambda = 0$.

In contrast, as shown in Fig. 1(b), the spectral measure μ_{11} associated with the time-dependent fluid velocity field in (1), with $\theta = 1$, has a large concentration of spectrum near the origin with significant values of $m_{11}(l) \gtrsim 10^{-10}$, more than *20 orders* of magnitude greater than that of the steady flow. A limit point behavior in the measure μ_{11} near $\lambda = 0$ can be seen in the rightmost panel of Fig. 1(b). Due to the significant mass of the measure near the spectral origin, the effective diffusivity has an $O(1)$ behavior, $S_{11}^* \sim 1$ for $\varepsilon \ll 1$, as shown in Fig. 1(d). This is consistent with numerical computations of S_{11}^* using alternate methods [15], showing that S_{11}^* plateaus off at ≈ 1.5 . The discrepancy between our result and that in [15] is likely due to finite size effects ($M = 20$) of our computation as well as the possibility of *continuous spectrum* at the spectral origin $\lambda = 0$ with significant measure mass. Although, our computation of S_{11}^* in Fig. 1(d) displays the correct qualitative behavior. These topics are part of future work.

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 [78, 86].

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 $\|\Phi^*\| = \|\Phi\|$ [78]. Consequently, Φ and its adjoint Φ^* have identical domains,

$$(32) \quad D(\Phi) = D(\Phi^*),$$

as they can be taken, without loss of generality [84], to be the entire Hilbert space, $D(\Phi) = D(\Phi^*) = \mathcal{H}$. The operator Φ is said to be *symmetric* if [78]

$$(33) \quad \langle \Phi\psi, \varphi \rangle = \langle \psi, \Phi\varphi \rangle, \text{ for all } \psi, \varphi \in D(\Phi).$$

By definition [78, 86], the two properties (32) and (33) 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} [78]. 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 [78, 86]. 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 [86]. Only for self-adjoint operators does the spectral theorem hold [78, 86].

The spectrum Σ of a self-adjoint operator Φ on a Hilbert space \mathcal{H} is real-valued [78, 86]. If Φ is bounded, then its spectral radius equal to its operator norm $\|\Phi\|$ [78], i.e.,

$$(34) \quad \Sigma \subseteq [-\|\Phi\|, \|\Phi\|].$$

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} [86].

We now summarize the spectral theorem for self-adjoint operators [86]. 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 [86]

$$(35) \quad \lim_{\lambda \rightarrow \inf \Sigma} Q(\lambda) = 0, \quad \lim_{\lambda \rightarrow \sup \Sigma} Q(\lambda) = I,$$

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 $\psi, \varphi \in D(\Phi)$ [86].

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

$$(36) \quad \operatorname{Re} \mu_{\psi\varphi}(\lambda) = \frac{1}{2} (\mu_{\psi\varphi}(\lambda) + \overline{\mu_{\psi\varphi}(\lambda)}), \quad \operatorname{Im} \mu_{\psi\varphi}(\lambda) = \frac{1}{2\imath} (\mu_{\psi\varphi}(\lambda) - \overline{\mu_{\psi\varphi}(\lambda)}),$$

where $\imath = \sqrt{-1}$, $\operatorname{Re} \mu_{\psi\psi}(\lambda) = \mu_{\psi\psi}(\lambda)$ and $\operatorname{Im} \mu_{\psi\psi}(\lambda) = 0$. With each of these strictly increasing functions of bounded variation, we associate Stieltjes measures [85, 86, 34]

$$(37) \quad \begin{aligned} d\mu_{\psi\varphi}(\lambda) &= d\langle Q(\lambda)\psi, \varphi \rangle, & d\operatorname{Re} \mu_{\psi\varphi}(\lambda) &= d\operatorname{Re} \langle Q(\lambda)\psi, \varphi \rangle, \\ d\mu_{\psi\psi}(\lambda) &= d\|Q(\lambda)\psi\|^2, & d\operatorname{Im} \mu_{\psi\varphi}(\lambda) &= d\operatorname{Im} \langle Q(\lambda)\psi, \varphi \rangle, \end{aligned}$$

which we will denote by $\mu_{\psi\psi}$, $\mu_{\psi\varphi}$, $\operatorname{Re} \mu_{\psi\varphi}$, and $\operatorname{Im} \mu_{\psi\varphi}$. We stress that $\mu_{\psi\psi}$ is a positive measure, $\mu_{\psi\varphi}$ is a complex measure, while $\operatorname{Re} \mu_{\psi\varphi}$ and $\operatorname{Im} \mu_{\psi\varphi}$ are signed measures [85, 86].

The spectral theorem also provides an operational calculus in Hilbert space which yields powerful integral representations involving the Stieltjes measures displayed in equation (37). 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 [86]

$$(38) \quad \begin{aligned} \langle F(\Phi)\psi, \varphi \rangle &= \int_{-\infty}^{\infty} F(\lambda) d\mu_{\psi\varphi}(\lambda), & \forall \psi \in \mathcal{D}(F), \varphi \in D(\Phi), \\ \langle F(\Phi)\psi, G(\Phi)\varphi \rangle &= \int_{-\infty}^{\infty} F(\lambda)\overline{G}(\lambda) d\mu_{\psi\varphi}(\lambda), & \forall \psi \in \mathcal{D}(F), \varphi \in \mathcal{D}(G), \end{aligned}$$

where the integration in (38) is over the spectrum Σ of Φ [78, 86].

The mass $\mu_{\psi\varphi}^0 = \int_{-\infty}^{\infty} d\mu_{\psi\varphi}(\lambda)$ of the Stieltjes measure $\mu_{\psi\varphi}$ satisfies [86] $\mu_{\psi\varphi}^0 = \lim_{\lambda \rightarrow \sup \Sigma} \mu_{\psi\varphi}(\lambda) - \lim_{\lambda \rightarrow \inf \Sigma} \mu_{\psi\varphi}(\lambda)$. Consequently, equation (35) yields

$$(39) \quad \mu_{\psi\varphi}^0 = \int_{-\infty}^{\infty} d\langle Q(\lambda)\psi, \varphi \rangle = \langle \psi, \varphi \rangle, \quad |\mu_{\psi\varphi}^0| \leq \|\psi\| \|\varphi\| < \infty.$$

Equation (39) demonstrates that the measures in (37) are *finite measures*, i.e., they have bounded mass [86].

Equation (38) can be generalized, holding with suitable notational changes, for *maximal normal operators* [86]. 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 $\mathbf{N} = \Phi_1 + \imath\Phi_2$, 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} [86]. A special case of a normal operator is a *skew-adjoint* operator satisfying $\mathbf{N}^* = -\mathbf{N}$. It can be decomposed as $\mathbf{N} = \imath\Phi_2$ and since Φ_2 is self-adjoint having purely real spectrum, the skew-adjoint operator $\mathbf{N} = \imath\Phi_2$ has purely imaginary spectrum [86]. Consequently, given such a maximal skew-adjoint operator, one can focus attention on the self-adjoint operator $\Phi_2 = -\imath\mathbf{N}$ 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 (37) arise naturally when considering a maximal skew-adjoint operator $\mathbf{N} = \imath\Phi$, 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,

$$(40) \quad \langle F(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle = \frac{1}{2}(\langle F(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle + \langle G(\mathbf{N})\varphi, F(\mathbf{N})\psi \rangle).$$

Now consider the special cases $F(\mathbf{N}) = G(\mathbf{N})$ and $F(\mathbf{N}) = \mathbf{N}G(\mathbf{N})$, i.e., $F(i\lambda) = G(i\lambda)$ and $F(i\lambda) = i\lambda G(i\lambda)$ in equation (38), respectively. It follows from equations (38) and (40), the identities $\operatorname{Re} z = (z + \bar{z})/2$ and $\operatorname{Im} z = (z - \bar{z})/(2i)$, and the linearity properties [86] of Stieltjes-Radon integrals with respect to the functions $\mu_{\psi\varphi}(\lambda)$ and $\bar{\mu}_{\psi\varphi}(\lambda)$ that

$$(41) \quad \begin{aligned} \langle G(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle &= \int_{-\infty}^{\infty} |G(i\lambda)|^2 d\operatorname{Re} \mu_{\psi\varphi}(\lambda), \\ \langle \mathbf{N}G(\mathbf{N})\psi, G(\mathbf{N})\varphi \rangle &= - \int_{-\infty}^{\infty} \lambda |G(i\lambda)|^2 d\operatorname{Im} \mu_{\psi\varphi}(\lambda). \end{aligned}$$

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 [86]

$$(42) \quad \langle \Phi\psi, \varphi \rangle = \int_{-\infty}^{\infty} \lambda d\mu_{\psi\varphi}(\lambda), \quad \|\Phi\psi\|^2 = \int_{-\infty}^{\infty} \lambda^2 d\mu_{\psi\psi}(\lambda),$$

where φ is an arbitrary element in $D(\Phi)$ [86]. In fact, this determines the one-to-one correspondence between the self-adjoint operator Φ and its resolution of the identity $Q(\lambda)$ [86].

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

$$(43) \quad \varphi_n(t) = \beta \sin(n\pi t/T), \quad \beta = \sqrt{2/T}, \quad \langle \varphi_n, \varphi_m \rangle_2 = \delta_{nm}, \quad n, m \in \mathbb{N},$$

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 [78, 86]. Consider the class $\mathcal{A}_{\mathcal{T}}$ of all functions $\psi \in L^2(\mathcal{T})$ such that $\psi(t)$ is *absolutely continuous* [79] on the interval \mathcal{T} and has a derivative $\psi'(t)$ belonging to $L^2(\mathcal{T})$, i.e., [86, 79]

$$(44) \quad \mathcal{A}_{\mathcal{T}} = \left\{ \psi \in L^2(\mathcal{T}) \mid \psi(t) = c + \int_0^t g(s)ds, \quad g \in L^2(\mathcal{T}) \right\},$$

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 (44) 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 (44) with $c = 0$ and $\int_0^T g(s)ds = 0$. More concisely,

$$(45) \quad \tilde{\mathcal{A}}_{\mathcal{T}} = \{\psi \in \mathcal{A}_{\mathcal{T}} \mid \psi(0) = \psi(T)\}, \quad \hat{\mathcal{A}}_{\mathcal{T}} = \{\psi \in \mathcal{A}_{\mathcal{T}} \mid \psi(0) = \psi(T) = 0\}.$$

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 $L^2(\mathcal{T})$ [86]. 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} [86]. 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 $\tilde{\mathcal{A}}_{\mathcal{T}}$ has a simple point spectrum, consisting of eigenvalues $\lambda = 2n\pi/T$, $n \in \mathbb{Z}$, with corresponding eigenfunctions $\exp(2n\pi t/T)$ [86].

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 [70], 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 D we use the one-to-one correspondence between a self-adjoint operator and its resolution of the identity [86], discussed in the paragraph containing equation (42), 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 $\mathcal{H}_{\mathcal{V}}$,

$$(46) \quad \mathcal{H}_{\mathcal{T}} = \{\psi \in L^2(\mathcal{T}) \mid \psi(t) = \psi(t+T)\}, \quad \mathcal{H}_{\mathcal{V}} = \{\psi \in L^2(\mathcal{V}) \mid \psi(\mathbf{x}) = \psi(\mathbf{x} + \ell \mathbf{e}_j)\},$$

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 $\|\psi\| = \langle \psi, \psi \rangle^{1/2}$ [34].

In equation (45) we defined the space $\tilde{\mathcal{A}}_{\mathcal{T}}$ 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 $\mathcal{H}_{\mathcal{T}}$ [86]. We now define the Sobolev space $\mathcal{H}_{\mathcal{V}}^1$, which is also a Hilbert space [13, 33, 59],

$$(47) \quad \mathcal{H}_{\mathcal{V}}^1 = \{\psi \in \mathcal{H}_{\mathcal{V}} \mid \langle |\nabla \psi|^2 \rangle_{\mathcal{V}} < \infty\},$$

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

$$(48) \quad \mathcal{H} = \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1, \quad \mathcal{F} = \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1.$$

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 $\mathcal{H} \equiv \mathcal{F} \equiv \mathcal{H}_V^1$.

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 (10) and (11), involving the solution χ_j of the cell problem in equation (9) 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 (9) yields

$$(49) \quad (-\Delta)^{-1}u_j = (\varepsilon + A)\chi_j,$$

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 $L^2(\mathcal{V})$ [84], hence \mathcal{H}_V^1 . Now write the functional $\langle u_j \chi_k \rangle$ in equation (10) as [70]

$$(50) \quad \langle u_j \chi_k \rangle = \langle [\Delta \Delta^{-1} u_j] \chi_k \rangle = -\langle \nabla \Delta^{-1} u_j \cdot \nabla \chi_k \rangle = \langle (-\Delta)^{-1} u_j, \chi_k \rangle_1.$$

This calculation will be rigorously justified in Theorem 1 below. Substituting the formula for $(-\Delta)^{-1}u_j$ in (49) into equation (50) yields equation (12), 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 (49) is equivalent to the resolvent formula displayed in equation (13). From equations (12) and (13) we have the functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* displayed in equation (14), 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 (14).

Theorem 1 *The operator $A = (-\Delta)^{-1}(\partial_t - \mathbf{u} \cdot \nabla)$ displayed in equation (12) is a maximal (skew-symmetric) normal operator on the function space \mathcal{F} defined in equation (48), hence $M = -iA$ is self-adjoint 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 (13) 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 (36). 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 (14) have the Radon–Stieltjes integral representations displayed in equation (15).*

Proof of Theorem 1. We first establish that $M = -\imath A$ is a self-adjoint operator on \mathcal{F} . The Sobelov space \mathcal{H}_V^1 in (47) 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 [13]. Furthermore, the elements of $\tilde{\mathcal{A}}_{\mathcal{T}}$ are those elements of $\mathcal{H}_{\mathcal{T}}$ that are differentiable almost everywhere (except on a set of Lebesgue measure zero), have square integrable derivatives on the interval \mathcal{T} , and are indefinite integrals of their derivative, hence continuous [79]. Consequently, $f \in \mathcal{F}$ implies that [86, 79]

$$(51) \quad \|f\|_{\infty} = \sup_{(t, \mathbf{x}) \in \mathcal{T} \times V} |f(t, \mathbf{x})| < \infty,$$

almost everywhere. For $u_j \in \mathcal{F}$ and fixed $t \in \mathcal{T}$, equation (51) implies that $[\mathbf{u}(t, \cdot) \cdot \nabla] : \mathcal{H}_V^1 \rightarrow \mathcal{H}_V$, while $(-\Delta)^{-1} : \mathcal{H}_V \rightarrow \mathcal{H}_V^1$ [13]. In particular, for $f, h \in \mathcal{F}$ we have that $\langle (-\Delta)^{-1} f, h \rangle_1 = \langle f, h \rangle$ [13]. This justifies the calculation in equation (50).

We have already established in Section B that the operator $-\imath \partial_t$ with domain $\tilde{\mathcal{A}}_{\mathcal{T}}$ is self-adjoint [86]. The integral operator $(-\Delta)^{-1}$ is self-adjoint and compact on \mathcal{H}_V [84]. Since they commute on $\tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_V$ [34], it follows that the operator $-\imath (-\Delta)^{-1} \partial_t$ is self-adjoint with domain $\tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_V$, hence $(-\Delta)^{-1} \partial_t$ is a maximal (skew-symmetric) normal operator on the same domain [86].

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 [13, 70]. Since the operator $(-\Delta)^{-1}$ is compact on \mathcal{H}_V [84], 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 (51) yields

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

This demonstrates that the operator norm $\|\mathbf{u} \cdot \nabla\|$ has the upper bounded $\|\mathbf{u} \cdot \nabla\| \leq \sqrt{d} \max_j \|u_j\|_\infty < \infty$ and establishes that $(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]$ is a compact operator on \mathcal{F} . Since $(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]$ is antisymmetric and bounded on \mathcal{F} , it is a maximal (skew-adjoint) normal operator on \mathcal{F} , hence $-i(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]$ is self-adjoint on \mathcal{F} [86].

Denote $M = -iA$, where $A = (-\Delta)^{-1}(\partial_t - \mathbf{u} \cdot \nabla)$. Since $-i(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]$ is a self-adjoint operator with domain containing \mathcal{F} and $-i(-\Delta)^{-1}\partial_t$ is self-adjoint with domain $\tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$, the operator M is self-adjoint with domain $D(M) \supset (\tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}) \cap \mathcal{F} = \mathcal{F}$ [86].

The complex-valued functions involved in the functional formulas for S_{jk}^* and A_{jk}^* in equation (14) are $F(\lambda) = (\varepsilon + i\lambda)^{-1}$ and $G(\lambda) = i\lambda(\varepsilon + i\lambda)^{-1}$. 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 (39), 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 $g_j = (-\Delta)^{-1}u_j \in \mathcal{F}$. We note that in the mean-zero setting, $\langle u_j \rangle = 0$ and the Fubini-Tonelli theorem [34] imply that we also have $\langle g_j \rangle = 0$. The conditions of the spectral theorem are thus satisfied. Consequently, the integral representations in equation (38) hold for the functions $F(\lambda)$ and $G(\lambda)$ defined above, involving the complex measure μ_{jk} . The discussion leading to equation (41) then establishes the integral representations for S_{jk}^* and A_{jk}^* displayed in equation (15).

It is worth noting that from equations (39) and (50), the mass μ_{jk}^0 of the measure μ_{jk} is given by $\mu_{jk}^0 = \langle g_j, g_k \rangle_1 = \langle (-\Delta)^{-1} u_j, u_k \rangle_2$, where $\langle \cdot, \cdot \rangle_2$ denotes the $L^2(\mathcal{T} \times \mathcal{V})$ inner-product. Since $(-\Delta)^{-1}$ is a self-adjoint operator on $L^2(\mathcal{V})$ [84], the spectral theorem demonstrates that

$$(53) \quad \mu_{jk}^0 = \langle (-\Delta)^{-1} u_j, u_k \rangle_2 = \int \lambda d\langle \tilde{Q}(\lambda) u_j, u_k \rangle_2.$$

In other words, the mass μ_{jk}^0 of the measure μ_{jk} is the first moment of the spectral measure $d\langle \tilde{Q}(\lambda) u_j, u_k \rangle_2$ of the self-adjoint operator $(-\Delta)^{-1}$, where $\tilde{Q}(\lambda)$ is the resolution of the identity in one-to-one correspondence with $(-\Delta)^{-1}$. This completes the proof of Theorem 1 \square .

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

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

$$(54) \quad \mathcal{U} = \{u_j \in \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}} \mid \exists 0 < C < \infty \text{ such that } \|(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]\| < C\}.$$

Corollary 2 states that the requirement $u_j \in \mathcal{F} = \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}^1$ can be weakened to $u_j \in \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$ such that the operator $(-\Delta)^{-1}[\mathbf{u} \cdot \nabla]$ is bounded on \mathcal{F} . The set \mathcal{U} in (54) is non-empty. We established this in (52), showing that $\{u_j \in \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}} \mid \|u_j\|_{\infty} < \infty\} \subset \mathcal{U}$, as $(-\Delta)^{-1}$ is a bounded operator on $\mathcal{H}_{\mathcal{V}}$ [84]. This extension of Theorem 1 allows for spatially *unbounded flows* with square integrable singularities.

Proof of Corollary 2. There are three places in the proof of Theorem 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 (50). The functional $\langle u_j \chi_k \rangle$ in equation (50) 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 (50) 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 $(-\Delta)^{-1} : \mathcal{H}_{\mathcal{V}} \rightarrow \mathcal{H}_{\mathcal{V}}^1$ [13]. 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 (38). Namely, that $(-\Delta)^{-1}u_j \in D(A) \supset \mathcal{F}$, as well as $(-\Delta)^{-1}u_j \in \mathcal{D}(F)$ and $(-\Delta)^{-1}u_j \in \mathcal{D}(G)$ for $F(\lambda) = (\varepsilon + \imath\lambda)^{-1}$ and $G(\lambda) = \imath\lambda(\varepsilon + \imath\lambda)^{-1}$. However, we demonstrated that $f \in \mathcal{D}(F)$ and $f \in \mathcal{D}(G)$ for all $f \in \mathcal{F}$. Since $(-\Delta)^{-1} : \mathcal{H}_{\mathcal{V}} \rightarrow \mathcal{H}_{\mathcal{V}}^1$ [13], we only require that $u_j \in \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}$. 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 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 (12)–(15) involving the *curl-free* vector field $\nabla\chi_j$ displayed in equation (9) 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 (46) and the function space $\tilde{\mathcal{A}}_{\mathcal{T}}$ given in equation (45). Now define their d -dimensional analogues over the complex field \mathbb{C} ,

$$(55) \quad \mathcal{H}_{\mathcal{T}} = \otimes_{j=1}^d \mathcal{H}_{\mathcal{T}}, \quad \mathcal{H}_{\mathcal{V}} = \otimes_{j=1}^d \mathcal{H}_{\mathcal{V}}, \quad \tilde{\mathcal{A}}_{\mathcal{T}} = \otimes_{j=1}^d \tilde{\mathcal{A}}_{\mathcal{T}}.$$

By the Helmholtz theorem [52, 11], 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 $\mathbf{\Gamma}_{\times} = -\nabla(-\Delta)^{-1}\nabla\cdot$, $\mathbf{\Gamma}_{\bullet} = \nabla \times (-\Delta)^{-1}\nabla \times$, and $\mathbf{\Gamma}_0 = \langle \cdot \rangle$, respectively, satisfying $\mathbf{I} = \mathbf{\Gamma}_{\times} + \mathbf{\Gamma}_{\bullet} + \mathbf{\Gamma}_0$ [29, 62]. 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{I} 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 (9), we will find particular use of the Hilbert space \mathcal{H}_{\times} , which we define as

$$(56) \quad \mathcal{H}_{\times} = \{\psi \in \mathcal{H}_{\mathcal{V}} \mid \mathbf{\Gamma}\psi = \psi \text{ weakly}\}, \quad \mathbf{\Gamma} = -\nabla(-\Delta)^{-1}\nabla\cdot,$$

where we have denoted $\mathbf{\Gamma}_{\times}$ by $\mathbf{\Gamma}$ for notational simplicity. Since $(-\Delta)^{-1}$ is self-adjoint on \mathcal{H}_{\times} [84], it is clear from integration by parts that $\mathbf{\Gamma}$ is a symmetric operator on \mathcal{H}_{\times} , and since it is also a projection operator, it is

bounded with operator norm $\|\mathbf{\Gamma}\| = 1$. Thus $\mathbf{\Gamma}$ is *self-adjoint* on \mathcal{H}_\times [86, 78]. Analogous to equation (48), we define the Hilbert space \mathcal{H} and its everywhere dense subset \mathcal{F} ,

$$(57) \quad \mathcal{H} = \mathcal{H}_\mathcal{T} \otimes \mathcal{H}_\times, \quad \mathcal{F} = \tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\times.$$

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 $\langle \psi, \varphi \rangle = \overline{\langle \varphi, \psi \rangle}$. 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]

$$(58) \quad \mathbf{u} = \nabla \cdot \mathbf{H}, \quad \mathbf{H}^T = -\mathbf{H},$$

where \mathbf{H}^T denotes transposition of the matrix \mathbf{H} . Since $\mathbf{u} \in \mathcal{F}$, we have that the space-time periodic components \mathbf{H}_{jk} of the matrix \mathbf{H} have square integrable spatial derivatives of order two on the set \mathcal{V} and are absolutely absolutely continuous with square integrable temporal derivatives on the set \mathcal{T} [13]. Consequently, as in (51), $\|\mathbf{H}_{jk}\|_\infty < \infty$ hence \mathbf{H} is bounded in operator norm $\|\mathbf{H}\| < \infty$ on $\mathcal{H}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$. 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 (58), the advection-diffusion equation in (2) can be written as a diffusion equation [29],

$$(59) \quad \partial_t \phi = \nabla \cdot \mathbf{D} \nabla \phi, \quad \phi(0, \mathbf{x}) = \phi_0(\mathbf{x}), \quad \mathbf{D} = \varepsilon \mathbf{I} + \mathbf{H},$$

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

$$(60) \quad D_{jk} = \varepsilon \delta_{jk} + H_{jk}, \quad j, k = 1, \dots, d.$$

The cell problem in (9) can also be written as the following diffusion equation [29]

$$(61) \quad \partial_\tau \chi_j = \nabla_\xi \cdot [\mathbf{D}(\nabla_\xi \chi_j + \mathbf{e}_j)], \quad \langle \nabla_\xi \chi_k \rangle = 0, \quad \mathbf{D} = \varepsilon \mathbf{I} + \mathbf{H},$$

where $\langle \nabla_\xi \chi_k \rangle = 0$ follows from the periodicity of χ_k . We stress that equation (59) involves the slow (t, \mathbf{x}) and fast variables $(\tau, \boldsymbol{\xi})$, while equation (61) involves only the fast variables. For notational simplicity, we will drop the subscripts ξ displayed in equation (61).

We now recast the first formula in equation (61) in a more suggestive, divergence form. Define the operator $\mathbf{T} : \tilde{\mathcal{A}}_{\mathcal{T}} \rightarrow \mathcal{H}_{\mathcal{T}}$ by $(\mathbf{T}\psi)_j = \partial_{\tau}\psi_j$, $j = 1, \dots, d$. For $f \in \mathcal{F}$ we have [29, 34, 33]

$$(62) \quad \nabla(\Delta^{-1})\partial_{\tau}f = \Delta^{-1}\mathbf{T}\nabla f,$$

so that [29] $\partial_{\tau}\chi_k = \Delta\Delta^{-1}\partial_{\tau}\chi_k = \nabla \cdot (\Delta^{-1}\mathbf{T})\nabla\chi_k$. Define the vector field $\mathbf{E}_k = \nabla\chi_k + \mathbf{e}_k$ and the operator $\sigma = \varepsilon\mathbf{I} + \mathbf{S}$, 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 $\mathbf{S} = \mathbf{H}$ and $\sigma = \mathbf{D}$. With these definitions, the cell problem in (61) can be written as $\nabla \cdot \sigma \mathbf{E}_k = 0$, $\langle \mathbf{E}_k \rangle = \mathbf{e}_k$, which is equivalent to

$$(63) \quad \nabla \cdot \mathbf{J}_k = 0, \quad \nabla \times \mathbf{E}_k = 0, \quad \mathbf{J}_k = \sigma \mathbf{E}_k, \quad \langle \mathbf{E}_k \rangle = \mathbf{e}_k, \quad \sigma = \varepsilon\mathbf{I} + \mathbf{S}.$$

The formulas in (63) are the quasi-static limit of Maxwell's equations for a conductive medium [36, 62], where \mathbf{E}_k and \mathbf{J}_k are the local electric field and current density, respectively, and σ is the local conductivity tensor of the medium. In the analytic continuation method for composites [36, 61, 9], the effective conductivity tensor σ^* is defined as

$$(64) \quad \langle \mathbf{J}_k \rangle = \sigma^* \langle \mathbf{E}_k \rangle.$$

The linear constitutive relation $\mathbf{J}_k = \sigma \mathbf{E}_k$ in (63) relates the local intensity and flux, while that in (64) relates the mean intensity and flux. Due to the skew-symmetry of \mathbf{S} , the intensity-flux relationship in (63) is similar to that of a Hall medium [43, 29]. The precise relationship between the effective parameters \mathbf{D}^* and σ^* are established in Lemma 4 below.

Analogous to equation (12), the components \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* , $j, k = 1, \dots, d$, of the symmetric \mathbf{S}^* and antisymmetric \mathbf{A}^* parts of the effective diffusivity tensor \mathbf{D}^* can be represented by the following functional formulas in terms of the \mathcal{H} -inner-product $\langle \cdot, \cdot \rangle$,

$$(65) \quad \mathbf{S}_{jk}^* = \varepsilon(\delta_{jk} + \langle \nabla\chi_j, \nabla\chi_k \rangle), \quad \mathbf{A}_{jk}^* = \langle \mathbf{A}\nabla\chi_j, \nabla\chi_k \rangle, \quad \mathbf{A} = \mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}.$$

Equation (65) follows from the formula $\mathbf{D}_{jk}^* = \varepsilon\delta_{jk} + \langle u_j \chi_k \rangle$ in equation (10) and the cell problem in equation (63) written as $\nabla \cdot \sigma \nabla\chi_j = -\nabla \cdot \mathbf{H}\mathbf{e}_j = -u_j$, yielding

$$(66) \quad \langle u_j \chi_k \rangle = -\langle [\nabla \cdot \sigma \nabla\chi_j], \chi_k \rangle = \langle \sigma \nabla\chi_j, \nabla\chi_k \rangle = \varepsilon\langle \nabla\chi_j, \nabla\chi_k \rangle + \langle \mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}\nabla\chi_j, \nabla\chi_k \rangle,$$

where we have used the periodicity of χ_k and \mathbf{H} in the second equality and the final equality follows from the property $\mathbf{\Gamma}\nabla\chi_j = \nabla\chi_j$. We stress that, since $\mathbf{\Gamma}$ is a projection on \mathcal{H} and therefore acts as the identity, we have the weak equality $\mathbf{A} = \mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma} = \mathbf{S}\mathbf{\Gamma} = \mathbf{\Gamma}\mathbf{S} = \mathbf{S}$.

Since $\nabla\chi_k$ is real-valued, we have that $\langle \nabla\chi_k, \nabla\chi_j \rangle = \langle \nabla\chi_j, \nabla\chi_k \rangle$, implying that \mathbf{S}^* is indeed a symmetric matrix. As in Section C.1, we have $(-\Delta)^{-1}\mathbf{T}\psi = \mathbf{T}(-\Delta)^{-1}\psi$ for $\psi \in \mathcal{F}$ [34, 84]. This and the skew-symmetry of the matrix \mathbf{H} implies that $\mathbf{S} = \mathbf{H} + (-\Delta)^{-1}\mathbf{T}$ is a skew-symmetric operator on \mathcal{F} . Since, $\mathbf{\Gamma}$ is self-adjoint on \mathcal{F} , $\mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}$ is also skew-symmetric on \mathcal{F} . Just as in Section C.1, this implies that \mathbf{A}^* is indeed an antisymmetric matrix. Analogous to equation (13) we have the following resolvent formula for $\nabla\chi_j$

$$(67) \quad \nabla\chi_j = (\varepsilon\mathbf{I} + \mathbf{A})^{-1}\mathbf{g}_j, \quad \mathbf{g}_j = -\mathbf{\Gamma}\mathbf{H}\mathbf{e}_j.$$

Equation (67) follows from applying the integro-differential operator $\nabla(\Delta^{-1})$ to the cell problem in equation (63) written as $\nabla \cdot \sigma \nabla \chi_j = -\nabla \cdot \mathbf{H}\mathbf{e}_j$, yielding

$$(68) \quad \mathbf{\Gamma}(\varepsilon\mathbf{I} + \mathbf{S})\nabla\chi_j = -\mathbf{\Gamma}\mathbf{H}\mathbf{e}_j.$$

The equivalence of equations (67) and (68) then follows from the formula $\mathbf{\Gamma}\nabla\chi_j = \nabla\chi_j$. Inserting the resolvent formula in (67) for $\nabla\chi_j$ into equation (65) yields the following analogue of (14)

$$(69) \quad \mathbf{S}_{jk}^* = \varepsilon \left(\delta_{jk} + \langle (\varepsilon\mathbf{I} + \mathbf{A})^{-1}\mathbf{g}_j, (\varepsilon\mathbf{I} + \mathbf{A})^{-1}\mathbf{g}_k \rangle \right), \quad \mathbf{A}_{jk}^* = \langle \mathbf{A}(\varepsilon\mathbf{I} + \mathbf{A})^{-1}\mathbf{g}_j, (\varepsilon\mathbf{I} + \mathbf{A})^{-1}\mathbf{g}_k \rangle,$$

We therefore have the following corollary of Theorem 1.

Corollary 3 *The operator $\mathbf{A} = \mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}$ with $\mathbf{S} = \mathbf{H} + (-\Delta)^{-1}\mathbf{T}$ displayed in equation (65) is a maximal (skew-symmetric) normal operator on the function space \mathcal{F} defined in (55), hence $\mathbf{M} = -\imath\mathbf{A}$ is self-adjoint on \mathcal{F} . Let $\mathbf{Q}(\lambda)$ be the resolution of the identity in one-to-one correspondence with \mathbf{M} . Define the complex valued function $\mu_{jk}(\lambda) = \langle \mathbf{Q}(\lambda)\mathbf{g}_j, \mathbf{g}_k \rangle$, $j, k = 1, \dots, d$, where $\mathbf{g}_j = -\mathbf{\Gamma}\mathbf{H}\mathbf{e}_j$ is defined in (67) and $\langle \cdot, \cdot \rangle$ 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 (36). Then, for $\mathbf{u}, \nabla\chi_j \in \mathcal{F}$ and all $0 < \varepsilon < \infty$, the functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* displayed in (69) have the Radon–Stieltjes integral representations displayed in equation (15).*

Proof of Corollary 3. We first establish that $\mathbf{M} = -\imath\mathbf{A}$, with $\mathbf{A} = \mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}$, is a self-adjoint operator on \mathcal{F} . Since $\mathbf{\Gamma} : \mathcal{H}_{\mathcal{V}} \rightarrow \mathcal{H}_{\times}$ is a projection,

it acts as the identity on \mathcal{H}_\times . We can therefore focus our analysis on the operator $\mathbf{S} = \mathbf{H} + (-\Delta)^{-1}\mathbf{T}$. As discussed above, since $\mathbf{u} \in \mathcal{F}$ and $\mathbf{u} = \nabla \cdot \mathbf{H}$, the skew-symmetric matrix \mathbf{H} is bounded in operator norm $\|\mathbf{H}\| < \infty$ with domain $\mathcal{H}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$, and is therefore a maximal (skew-symmetric) normal operator, hence $-i\mathbf{H}$ is self-adjoint on the same domain [86]. It is clear from Section B that $-i\mathbf{T}$ is self-adjoint with domain $\tilde{\mathcal{A}}_\mathcal{T}$. The integral operator $(-\Delta)^{-1}$ is self-adjoint and compact on $\mathcal{H}_\mathcal{V}$. Since they commute on $\tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$ [34], it follows that the operator $-i(-\Delta)^{-1}\mathbf{T}$ is self-adjoint with domain $\tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$, hence $(-\Delta)^{-1}\mathbf{T}$ is a maximal (skew-symmetric) normal operator on the same domain. Since $-i\mathbf{H}$ is a self-adjoint operator with domain $\mathcal{H}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$ and $(-\Delta)^{-1}\mathbf{T}$ is self-adjoint with domain $\tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$, the operator $\mathbf{S} = \mathbf{H} + (-\Delta)^{-1}\mathbf{T}$ is self-adjoint with domain $D(\mathbf{S}) = \mathcal{H}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V} \cap \tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V} = \tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$ [86]. Consequently, the operator $\mathbf{M} = -i\mathbf{A}$, with $\mathbf{A} = \mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}$ is self-adjoint with domain $\mathcal{F} = \tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\times$.

In Theorem 1 we established that the functions $F(\lambda) = (\varepsilon + i\lambda)^{-1}$ and $G(\lambda) = i\lambda(\varepsilon + i\lambda)^{-1}$ involved in the functional formulas for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* in equation (69) are uniformly bounded for all $0 < \varepsilon < \infty$, so that $\varphi \in \mathcal{D}(F)$ and $\varphi \in \mathcal{D}(G)$ for all $\varphi \in D(\mathbf{M})$ when $0 < \varepsilon < \infty$. Since $\mathbf{g}_j = -\mathbf{\Gamma}\mathbf{H}\mathbf{e}_j$ and $\|\mathbf{g}_j\| \leq \|\mathbf{\Gamma}\|\|\mathbf{H}\| < \infty$, it is clear that $\mathbf{g}_j \in \mathcal{F} \subset D(\mathbf{M})$. In the setting of a mean-zero velocity field, $\mathbf{H}(t, \mathbf{x})$ is mean-zero in time. Consequently, $\langle \mathbf{g}_j \rangle = 0$ follows from the Fubini-Tonelli theorem [34]. The conditions of the spectral theorem are thus satisfied which, from the proof of Theorem 1, establishes the integral representations for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* displayed in equation (15). From equation (39), the mass μ_{jk}^0 of the measure μ_{jk} is given by

$$(70) \quad \mu_{jk}^0 = \langle \mathbf{g}_j, \mathbf{g}_k \rangle = \langle \mathbf{\Gamma}\mathbf{H}\mathbf{e}_j, \mathbf{\Gamma}\mathbf{H}\mathbf{e}_k \rangle = \langle -\mathbf{H}^T \mathbf{\Gamma}\mathbf{H}\mathbf{e}_j, \mathbf{e}_k \rangle.$$

Moreover, $|\mu_{jk}^0| \leq \|\mathbf{H}\|^2 < \infty$ for all $j, k = 1, \dots, d$. This completes the proof of Theorem 1 \square .

We conclude this section with the following lemma, which provides the relationship between the effective parameter $\boldsymbol{\sigma}^*$ defined in equation (64) and \mathbf{D}^* defined in (10).

Lemma 4 *Let the components \mathbf{D}_{jk}^* and σ_{jk}^* , $j, k = 1, \dots, d$, of the effective tensors \mathbf{D}^* and $\boldsymbol{\sigma}^*$ be defined as in equations (4)–(10) and (61)–(64), respectively. Then these effective tensors related by*

$$(71) \quad \boldsymbol{\sigma}^* = [\mathbf{D}^*]^T + \langle \mathbf{H} \rangle.$$

Proof of Lemma 4. Recall the definition of the function space $\mathcal{F} = \tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\times$ in (57), which we will denote by \mathcal{F}_\times here. Denote by $\mathcal{F}_\bullet = \tilde{\mathcal{A}}_\mathcal{T} \otimes \mathcal{H}_\bullet$,

where $\mathcal{H}_\bullet \subset \mathcal{H}_\mathcal{V}$ is the space of divergence-free fields. Recall that $\boldsymbol{\sigma} = \varepsilon \mathbf{I} + \mathbf{S}$ where $\mathbf{S} = \mathbf{H} + (-\boldsymbol{\Delta})^{-1} \mathbf{T}$. From equation (63) we have that $\mathbf{J}_k = \boldsymbol{\sigma} \mathbf{E}_k$ and $\mathbf{E}_k = \nabla \chi_k + \mathbf{e}_k$ satisfy $\mathbf{J}_k \in \mathcal{F}_\bullet$ and $\mathbf{E}_k \in \mathcal{F}_\times$. By the mutual orthogonality of the Hilbert spaces \mathcal{H}_\times and \mathcal{H}_\bullet we have that $\langle \mathbf{J}_j \cdot \nabla \chi_k \rangle = 0$ for all $j, k = 1, \dots, d$, which is equivalent to equation (66). Consequently, from equation (64) we have $\langle \mathbf{J}_j \cdot \mathbf{E}_k \rangle = \langle \mathbf{J}_j \cdot \mathbf{e}_k \rangle = \sigma_{jk}^*$.

From $\mathbf{S} = \mathbf{H} - (\boldsymbol{\Delta}^{-1}) \mathbf{T}$ we have $\mathbf{S} \mathbf{e}_j = \mathbf{H} \mathbf{e}_j$. By the definition $\mathbf{u} = \nabla \cdot \mathbf{H}$ in (58) and the periodicity of \mathbf{H} and χ_k , we also have $\langle \mathbf{H} \mathbf{e}_j \cdot \nabla \chi_k \rangle = -\langle u_j \chi_k \rangle$ via integration by parts. Therefore, by the skew-symmetry of \mathbf{S} on \mathcal{F}_\times , $\langle \nabla \chi_j \rangle = 0$, and equation (10), we have

$$\begin{aligned}
 (72) \quad \sigma_{jk}^* &= \langle \mathbf{J}_j \cdot \mathbf{e}_k \rangle \\
 &= \langle (\varepsilon \mathbf{I} + \mathbf{S}) \nabla \chi_j \cdot \mathbf{e}_k \rangle + \langle (\varepsilon \mathbf{I} + \mathbf{S}) \mathbf{e}_j \cdot \mathbf{e}_k \rangle \\
 &= -\langle \nabla \chi_j \cdot \mathbf{H} \mathbf{e}_k \rangle + \langle (\varepsilon \mathbf{I} + \mathbf{H}) \mathbf{e}_j \cdot \mathbf{e}_k \rangle \\
 &= \langle u_k \chi_j \rangle + \varepsilon \delta_{jk} + \langle \mathbf{H}_{jk} \rangle \\
 &= D_{kj}^* + \langle \mathbf{H}_{jk} \rangle,
 \end{aligned}$$

which is equivalent to equation (71). This concludes our proof of Lemma 4 \square .

Appendix D. An isometric correspondence

A natural question to ask is the following. Is the formulation of the effective parameter problem described in Theorem 1 equivalent to that described in Corollary 3? The answer is in the affirmative. The correspondence between the two formulations is one of isometry, and is summarized by the following theorem.

Theorem 5 *The function spaces \mathcal{F} and \mathcal{F} defined in equations (48) and (57) are in one-to-one isometric correspondence. This induces a one-to-one isometric correspondence between the domains $D(A)$ and $D(\mathbf{A})$ of the operators A and \mathbf{A} defined in equations (12) and (65), respectively. Specifically, for every $f \in D(A) \cap \mathcal{F}$ we have $\nabla f \in D(\mathbf{A}) \cap \mathcal{F}$ and $\|Af\|_1 = \|\mathbf{A}\nabla f\|$, and conversely, for each $\psi \in D(\mathbf{A}) \cap \mathcal{F}$ there exists unique $f \in D(A) \cap \mathcal{F}$ such that $\psi = \nabla f$ and $\|\mathbf{A}\psi\| = \|Af\|_1$. The Radon–Stieltjes measures underlying the integral representations of Theorem 1 and Corollary 3 are equal, $d\langle Q(\lambda)g_j, g_k \rangle_1 = d\langle \mathbf{Q}(\lambda)\mathbf{g}_j, \mathbf{g}_k \rangle$, $j, k = 1, \dots, d$, 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 $\mathbf{Q}(\lambda)\nabla = \nabla Q(\lambda)$.*

Proof of Theorem 5. We use the formula $\mathbf{u} = \nabla \cdot \mathbf{H}$ displayed in equation (58) and the identities $[\nabla \cdot \mathbf{H}] \cdot \nabla f = \nabla \cdot [\mathbf{H} \nabla f]$ and $[\nabla \cdot \mathbf{H}] \cdot \mathbf{e}_j = \nabla \cdot [\mathbf{H} \mathbf{e}_j]$ to write the operator $A = (-\Delta)^{-1}(\partial_t - \mathbf{u} \cdot \nabla)$ and function $g_j = (-\Delta)^{-1}u_j$ defined in equations (12) and (13) as $A = (-\Delta)^{-1}(\partial_t - \nabla \cdot \mathbf{H} \nabla)$ 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 $\nabla \Delta^{-1} \partial_t = \Delta^{-1} \mathbf{T} \nabla$, $\mathbf{A} = \mathbf{\Gamma} \mathbf{H} - \Delta^{-1} \mathbf{T}$, and $\mathbf{g}_j = -\mathbf{\Gamma} \mathbf{H} \mathbf{e}_j$, displayed in equations, (62), (65) and (67), respectively, we have that

$$(73) \quad \nabla A = [\Delta^{-1} \mathbf{T} - \mathbf{\Gamma} \mathbf{H}] \nabla = \mathbf{A} \nabla, \quad \nabla g_j = \mathbf{g}_j.$$

Consequently, by applying the differential operator ∇ to both sides of the formula $(\varepsilon + A)\chi_j = g_j$ of (13), we obtain the formula $(\varepsilon \mathbf{I} + \mathbf{A})\nabla \chi_j = \mathbf{g}_j$ of equation (67).

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 $\mathcal{H}_{\mathcal{V}}^1$ and \mathcal{H}_{\times} defined in equations (47) and (56), respectively. We will temporarily denote the inner-product induced norms of these Hilbert spaces by $\|\cdot\|_1$ and $\|\cdot\|$, respectively. The Sobelov space $\mathcal{H}_{\mathcal{V}}^1$ in (47) is the closure in the norm $\|\cdot\|_1$ of the space $C^2(\mathcal{V})$ of all twice continuously differentiable periodic functions in $\mathcal{H}_{\mathcal{V}}$ [13]. Functions in $\mathcal{H}_{\mathcal{V}}^1$ need not be differentiable in the classical sense. Instead, $f \in \mathcal{H}_{\mathcal{V}}^1$ has derivatives $\partial^k f / \partial x_j^k \in L^2(\mathcal{V})$ for $k = 1, 2$, defined by $\partial^k f / \partial x_j^k = \lim_{n \rightarrow \infty} \partial^k f_n / \partial x_j^k$ where $f_n \in C^2(\mathcal{V})$ are Cauchy in the norm $\|\cdot\|_1$ and converge to f in $L^2(\mathcal{V})$ [59].

Let $\{f_n\}$ be such a Cauchy sequence, i.e., for all $\epsilon > 0$, there exists an $N \in \mathbb{N}$ such that for all $n, m > N$ we have that $\|f_n - f_m\|_1 < \epsilon$ and $\lim_{n \rightarrow \infty} f_n = f$, where $f \in \mathcal{H}_{\mathcal{V}}^1$. Since $f_n \in C^2(\mathcal{V})$ and f_n is also \mathcal{V} -periodic, we have that $\Delta^{-1} \Delta f_n = f_n$ [59]. Consequently,

$$(74) \quad \epsilon > \|f_n - f_m\|_1 = \|\nabla \Delta^{-1} \Delta f_n - \nabla f_m\| = \|\mathbf{\Gamma} \nabla f_n - \nabla f_m\|,$$

which implies that $\mathbf{\Gamma} \nabla f = \nabla f$. Moreover, $\|\nabla f\|^2 = \langle \nabla f, \nabla f \rangle = \|f\|_1^2 < \infty$. 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 $\|f\|_1^2 = \langle \psi, \psi \rangle = \|\psi\|^2 < \infty$ 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 $\mathcal{F} \sim \mathcal{F}$.

We now return to our previous notation, where $\|\cdot\|_1$ and $\|\cdot\|$ denotes the norm induced by the \mathcal{H} -inner-product and \mathcal{H} -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} . This, in turn, follows from the one-to-one correspondence between a self-adjoint operator and its resolution of the identity discussed in Section A, leading to equation (42). More specifically, the domain $D(M)$ of the self-adjoint operator M , for example, comprises those and only those elements f of \mathcal{H} such that the Stieltjes integral $\int \lambda^2 d\|Q(\lambda)f\|_1^2$ is convergent, and when $f \in D(M)$ the element Mf is determined by the relations in equation (42). Since $A = \iota M$ it is clear that $D(A) = D(M)$. We already established in Section C.1 that $\mathcal{F} \subset D(A)$, and similarly for the operator \mathbf{A} .

Let $f \in D(A) \cap \mathcal{F}$. From the relation $\mathcal{F} \sim \mathcal{F}$, we have that $\nabla f \in \mathcal{F}$, so from equation (73)

$$(75) \quad \|Af\|_1^2 = \langle Af, Af \rangle_1 = \langle \nabla Af \cdot \nabla Af \rangle = \langle \mathbf{A} \nabla f \cdot \mathbf{A} \nabla f \rangle = \|\mathbf{A} \nabla f\|^2.$$

Consequently, from equation (42) we have that

$$(76) \quad \int \lambda^2 d\|Q(\lambda)f\|_1^2 = \int \lambda^2 d\|\mathbf{Q}(\lambda)\nabla f\|^2,$$

and the convergence of the integral on the left-hand-side of (76) implies the convergence of the integral on the right-hand-side which, in turn, implies that $\nabla f \in D(\mathbf{A})$.

Conversely, let $\psi \in D(\mathbf{A}) \cap \mathcal{F}$. From the relation $\mathcal{F} \sim \mathcal{F}$, there exists unique $f \in \mathcal{F}$ such that $\psi = \nabla f$, and equation (73) then implies that

$$(77) \quad \|\mathbf{A}\psi\|^2 = \langle \mathbf{A}\nabla f, \mathbf{A}\nabla f \rangle = \langle \nabla Af, \nabla Af \rangle = \langle Af, Af \rangle_1 = \|Af\|_1^2.$$

Again, equation (42) implies that (76) holds, and the convergence of the integral on the right-hand-side of (76) implies the convergence of the integral on the left-hand-side which, in turn, implies that $f \in D(A)$.

In summary, for every $f \in D(A) \cap \mathcal{F}$ we have $\nabla f \in D(\mathbf{A})$ and $\|Af\|_1^2 = \|\mathbf{A}\nabla f\|^2$. Conversely, for every $\psi \in D(\mathbf{A}) \cap \mathcal{F}$, there exists unique $f \in D(A)$ such that $\psi = \nabla f$ and $\|\mathbf{A}\psi\|^2 = \|Af\|_1^2$. This generates a one-to-one isometric correspondence between the domains $D(\mathbf{A})$ and $D(A)$.

We now show that this result implies, and is implied by the weak equality $\nabla Q(\lambda) = \mathbf{Q}(\lambda)\nabla$, where $Q(\lambda)$ and $\mathbf{Q}(\lambda)$ are the resolutions of the identity in one-to-one correspondence with the operators A and \mathbf{A} , respectively. From

equation (76) and the linearity properties of Radon–Stieltjes integrals [86], we have that

$$(78) \quad 0 = \int_{-\infty}^{\infty} \lambda^2 d(\|Q(\lambda)f\|_1^2 - \|\mathbf{Q}(\lambda)\nabla f\|^2) = \int_{-\infty}^{\infty} \lambda^2 d(\langle [\nabla Q(\lambda) - \mathbf{Q}(\lambda)\nabla]f \cdot \nabla f \rangle).$$

Equation (78) implies that for all $f \in D(A) \cap \mathcal{F} \iff \nabla f \in D(\mathbf{A}) \cap \mathcal{F}$ we have $d\|Q(\lambda)f\|_1^2 = d\|\mathbf{Q}(\lambda)\nabla f\|^2$, up to sets of measure zero. Moreover, the equality $\nabla Q(\lambda) = \mathbf{Q}(\lambda)\nabla$ holds in this weak sense. Conversely, assume that $Q(\lambda)$ and $\mathbf{Q}(\lambda)$ are the resolutions of the identity in one-to-one correspondence with the operators A and \mathbf{A} and that $\nabla Q(\lambda)f = \mathbf{Q}(\lambda)\nabla f$ for every $f \in D(A) \cap \mathcal{F} \iff \nabla f \in D(\mathbf{A}) \cap \mathcal{F}$. Then equation (78) holds and implies equation (76). Equation (42) then implies that $\|\mathbf{A}\nabla f\|^2 = \|Af\|_1^2 = \|\nabla Af\|^2$, which implies that $\mathbf{A}\nabla = \nabla A$ in this weak sense. 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 1 are equal to that of Corollary 3 $d\|Q(\lambda)g_k\|_1 = d\|\mathbf{Q}(\lambda)\mathbf{g}_k\|$ up to null sets of measure zero, for all $j, k = 1, \dots, d$. This concludes our proof of Theorem 5 \square .

D.1. Discrete integral representations by eigenfunction expansion

The integral representations of Theorem 1 and Corollary 3 displayed in equation (15), involve a spectral measure μ_{jk} , $j, k = 1, \dots, d$, which has discrete and continuous components [78, 86]. In this section, we review these properties of μ_{jk} and provide an explicit formula for its discrete component. Towards this goal, we summarize some general spectral properties of the self-adjoint operators $M = -\imath A$ and $\mathbf{M} = -\imath \mathbf{A}$ on the function spaces \mathcal{F} and \mathcal{H} , which are densely defined on the associated Hilbert spaces \mathcal{H} and \mathcal{H} , given in equations (48) and (57), respectively. We will focus on the operator M and the Hilbert space \mathcal{H} , as the discussion regarding \mathbf{M} and \mathcal{H} is analogous.

Recall from equation (42) that the domain $D(M)$ of the self-adjoint operator M comprises those and only those elements $f \in \mathcal{H}$ such that $\|Mf\|_1^2 = \int_{-\infty}^{\infty} \lambda^2 d\|Q(\lambda)f\|_1^2 < \infty$, where $Q(\lambda)$ is the resolution of the identity in one-to-one correspondence with M [86]. The integration is over the spectrum Σ of M , which has continuous Σ_{cont} and discrete (pure-point) Σ_{pp} components, $\Sigma = \Sigma_{\text{cont}} \cup \Sigma_{\text{pp}}$ [78, 86]. We first focus on the discrete spectrum Σ_{pp} .

The $f \in \mathcal{H}$, $f \neq 0$, satisfying $Mf = \lambda f$ with $\lambda \in \Sigma_{\text{pp}}$ are called eigenfunctions and λ is the corresponding eigenvalue. Since M is self-adjoint, λ

is real-valued [86]. The span of all eigenfunctions is a *countable* subspace of \mathcal{H} [86]. Accordingly, we will denote the eigenfunctions by φ_l , $l = 1, 2, 3, \dots$, with corresponding eigenvalues λ_l . Eigenfunctions corresponding to distinct eigenvalues are orthogonal and can be normalized to be orthonormal [86], i.e. if $M\varphi_l = \lambda_l\varphi_l$ and $M\varphi_m = \lambda_m\varphi_m$ for $\lambda_l \neq \lambda_m$, then $\langle \varphi_m, \varphi_n \rangle_1 = \delta_{mn}$. There can be more than one eigenfunction associated with a particular eigenvalue. However, they are linearly independent and, without loss of generality, can be taken to be orthonormal [86]. Consequently, associated with each eigenfunction φ_l is a closed linear manifold, which we denote by $\mathcal{M}(\varphi_l)$. When $l \neq m$, $\mathcal{M}(\varphi_l)$ and $\mathcal{M}(\varphi_m)$ are mutually orthogonal. Set $\mathcal{E} = \bigoplus_{l=1}^{\infty} \mathcal{M}(\varphi_l)$, $\mathcal{M} = \mathcal{E} \oplus \{0\}$, and let $\mathcal{N} = \mathcal{M}^{\perp}$ be the orthogonal complement of \mathcal{M} in \mathcal{H} . All the properties of \mathcal{M} and \mathcal{N} that are relevant here have been collected in the following theorem [86], which provides a natural decomposition of the Hilbert space \mathcal{H} in terms of the mutually orthogonal, closed linear manifolds \mathcal{M} and \mathcal{N} , and leads to a decomposition of the measure μ_{kk} into its discrete and continuous components.

Theorem 6 ([86] pages 189 and 247) *One of the three cases must occur:*

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

$$\mathcal{M} = \bigoplus_{l=1}^{\infty} \mathcal{M}(\varphi_l), \quad \mathcal{N} = \bigoplus_{m=1}^{\infty} \mathcal{N}(\psi_m), \quad \mathcal{H} = \mathcal{M} \oplus \mathcal{N}.$$

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

In each of these three cases, the closed linear manifolds \mathcal{M} and \mathcal{N} reduce M , i.e., M leaves both \mathcal{M} and \mathcal{N} invariant in the sense that if $f \in D(M)$ and $f \in \mathcal{N}$ then $Mf \in \mathcal{N}$, and similarly for \mathcal{M} . In cases (2) and (3), a necessary and sufficient condition that an element $\varphi_l \in \mathcal{H}$ be an eigenfunction with

eigenvalue λ_l , is that the function $\|Q(\lambda)\varphi_l\|_1^2$ is constant on each of the intervals $-\infty < \lambda < \lambda_l$ and $\lambda_l < \lambda < \infty$ [86]. Moreover, a necessary and sufficient condition that $f \in \mathcal{M}$, $f \neq 0$, is

$$(79) \quad f = \sum_{l=1}^{\infty} \langle f, \varphi_l \rangle_1 \varphi_l, \quad \|f\|_1^2 = \sum_{l=1}^{\infty} |\langle f, \varphi_l \rangle_1|^2 \neq 0,$$

and similarly for $f \in \mathcal{N}$ with orthonormal set $\{\psi_m\}$. In cases (1) and (2), a necessary and sufficient condition that $\psi \neq 0$ be an element of \mathcal{N} is that $\|Q(\lambda)\psi\|_1^2$ be a continuous function of λ not identically zero [86].

Let f be an arbitrary element of \mathcal{H} , and g and h be its (unique) projections on \mathcal{M} and \mathcal{N} , respectively, then the equation

$$(80) \quad \|Q(\lambda)f\|_1^2 = \|Q(\lambda)g\|_1^2 + \|Q(\lambda)h\|_1^2, \quad d\|Q(\lambda)f\|_1^2 = d\|Q(\lambda)g\|_1^2 + d\|Q(\lambda)h\|_1^2$$

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.

We now use the mathematical framework summarized in Theorem 6 to provide explicit formulas for the discrete parts of the integral representations for \mathbf{S}_{jk}^* and \mathbf{A}_{jk}^* , displayed in equation (15). Recall the cell problem in equation (9) written as in (49), $(\varepsilon + A)\chi_j = g_j$. Here $A = \imath M$ is defined in (12), $g_j = (-\Delta)^{-1}u_j$, and u_j is the j^{th} component of the velocity field \mathbf{u} , $j = 1, \dots, d$. Moreover, we have $\chi_j, g_j \in \mathcal{F} \subset \mathcal{H}$ and $\mathcal{F} \subset D(A)$. We stress that the arguments presented here are more subtle than those typically used for *bounded* operators in Hilbert space. The reason being is that a bounded linear operator commutes with all the infinite sums encountered here, by the dominated convergence theorem [34]. However, for the operator A , we must instead rely on general principles of unbounded linear operators in Hilbert space.

Let $\tilde{\chi}_j$ and χ_j^\perp be the (unique) projections of χ_j on \mathcal{M} and \mathcal{N} , respectively, with $\chi_j = \tilde{\chi}_j + \chi_j^\perp$ and similarly for g_j . Since $A = \imath M$ is a linear operator, we have that $A\chi_j = A\tilde{\chi}_j + A\chi_j^\perp$. From Theorem 6, the linear manifolds \mathcal{M} and \mathcal{N} both reduce A , which implies that $A\tilde{\chi}_j \in \mathcal{M}$ and $A\chi_j^\perp \in \mathcal{N}$. From equation (79) we then have $A\tilde{\chi}_j = \sum_l \langle A\tilde{\chi}_j, \varphi_l \rangle_1 \varphi_l$ and

$$(81) \quad \chi_j = \sum_l \langle \tilde{\chi}_j, \varphi_l \rangle_1 \varphi_l + \chi_j^\perp, \quad A\chi_j = \sum_l \imath \lambda_l \langle \tilde{\chi}_j, \varphi_l \rangle_1 \varphi_l + A\chi_j^\perp$$

where we have used that $\langle A\tilde{\chi}_j, \varphi_l \rangle_1 = -\langle \tilde{\chi}_j, A\varphi_l \rangle_1 = -\langle \tilde{\chi}_j, \imath\lambda_l\varphi_l \rangle_1 = \imath\lambda_l\langle \tilde{\chi}_j, \varphi_l \rangle_1$. From the cell problem $(\varepsilon + A)\chi_j = g_j$ we therefore have

$$(82) \quad \varepsilon \sum_l \langle \tilde{\chi}_j, \varphi_l \rangle_1 \varphi_l + \sum_l \imath\lambda_l \langle \tilde{\chi}_j, \varphi_l \rangle_1 \varphi_l + (\varepsilon + A)\chi_j^\perp = \tilde{g}_j + g_j^\perp,$$

where $(\varepsilon + A)\chi_j^\perp, g_j^\perp \in \mathcal{N}$. Of course, each $f \in \mathcal{N}$ can be represented [86] as $f = \sum_m \langle f, \psi_m \rangle_1 \psi_m$, where $\{\psi_m\}$ is the orthonormal set defined in Theorem 6, though we have suppressed this notation in the above equations for simplicity. By the mutual orthogonality of the linear manifolds \mathcal{M} and \mathcal{N} , the completeness of the set $\{\varphi_l\} \cup \{\psi_m\}$, and the Parseval identity, taking the inner-product of both sides of equation (82) with φ_n yields

$$(83) \quad \langle \tilde{\chi}_j, \varphi_n \rangle_1 = \frac{\langle \tilde{g}_j, \varphi_n \rangle_1}{\varepsilon + \imath\lambda_n}, \quad 0 < \varepsilon < \infty.$$

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 (12). Writing $\chi_j = \tilde{\chi}_j + \chi_j^\perp$ and $A\chi_j = A\tilde{\chi}_j + A\chi_j^\perp$, the mutual orthogonality of the linear manifolds \mathcal{M} and \mathcal{N} , which both reduce A , implies that $\langle \chi_j, \chi_k \rangle_1 = \langle \tilde{\chi}_j, \tilde{\chi}_k \rangle_1 + \langle \chi_j^\perp, \chi_k^\perp \rangle_1$ and $\langle A\chi_j, \chi_k \rangle_1 = \langle A\tilde{\chi}_j, \tilde{\chi}_k \rangle_1 + \langle A\chi_j^\perp, \chi_k^\perp \rangle_1$. Consequently, from equations (81) and (83), the completeness of the set $\{\varphi_l\} \cup \{\psi_m\}$, and the Parseval identity, we have

$$(84) \quad \begin{aligned} \langle \chi_j, \chi_k \rangle_1 - \langle \chi_j^\perp, \chi_k^\perp \rangle_1 &= \sum_l \langle \tilde{\chi}_j, \varphi_l \rangle_1 \overline{\langle \tilde{\chi}_k, \varphi_l \rangle_1} = \sum_l \frac{\langle \tilde{g}_j, \varphi_l \rangle_1 \overline{\langle \tilde{g}_k, \varphi_l \rangle_1}}{\varepsilon^2 + \lambda_l^2} \\ \langle A\chi_j, \chi_k \rangle_1 - \langle A\chi_j^\perp, \chi_k^\perp \rangle_1 &= \sum_l \imath\lambda_l \langle \tilde{\chi}_j, \varphi_l \rangle_1 \overline{\langle \tilde{\chi}_k, \varphi_l \rangle_1} = \sum_l \frac{\imath\lambda_l \langle \tilde{g}_j, \varphi_l \rangle_1 \overline{\langle \tilde{g}_k, \varphi_l \rangle_1}}{\varepsilon^2 + \lambda_l^2}. \end{aligned}$$

Since χ_j and $A\chi_j$ are real-valued, just as in equation (41), we have that

$$(85) \quad \begin{aligned} \langle \chi_j, \chi_k \rangle_1 - \langle \chi_j^\perp, \chi_k^\perp \rangle_1 &= \sum_l \frac{\operatorname{Re} [\langle \tilde{g}_j, \varphi_l \rangle_1 \overline{\langle \tilde{g}_k, \varphi_l \rangle_1}]}{\varepsilon^2 + \lambda_l^2} \\ \langle A\chi_j, \chi_k \rangle_1 - \langle A\chi_j^\perp, \chi_k^\perp \rangle_1 &= -\sum_l \frac{\lambda_l \operatorname{Im} [\langle \tilde{g}_j, \varphi_l \rangle_1 \overline{\langle \tilde{g}_k, \varphi_l \rangle_1}]}{\varepsilon^2 + \lambda_l^2}. \end{aligned}$$

The right hand sides of the formulas in equation (85) 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 $d\langle Q(\lambda)g_j^\perp, g_k^\perp \rangle_1$ via equation (15). We note that from the decomposition $g_j = \tilde{g}_j + g_j^\perp$, we have $\langle \tilde{g}_j, \varphi_l \rangle_1 = \langle g_j, \varphi_l \rangle_1$. A useful property of the inner-product $\langle g_j, \varphi_l \rangle_1$ and the form of $g_j = (-\Delta)^{-1}u_j$ is that (see equation (50))

$$(86) \quad \langle g_j, \varphi_l \rangle_1 = \langle u_j, \varphi_l \rangle_2.$$

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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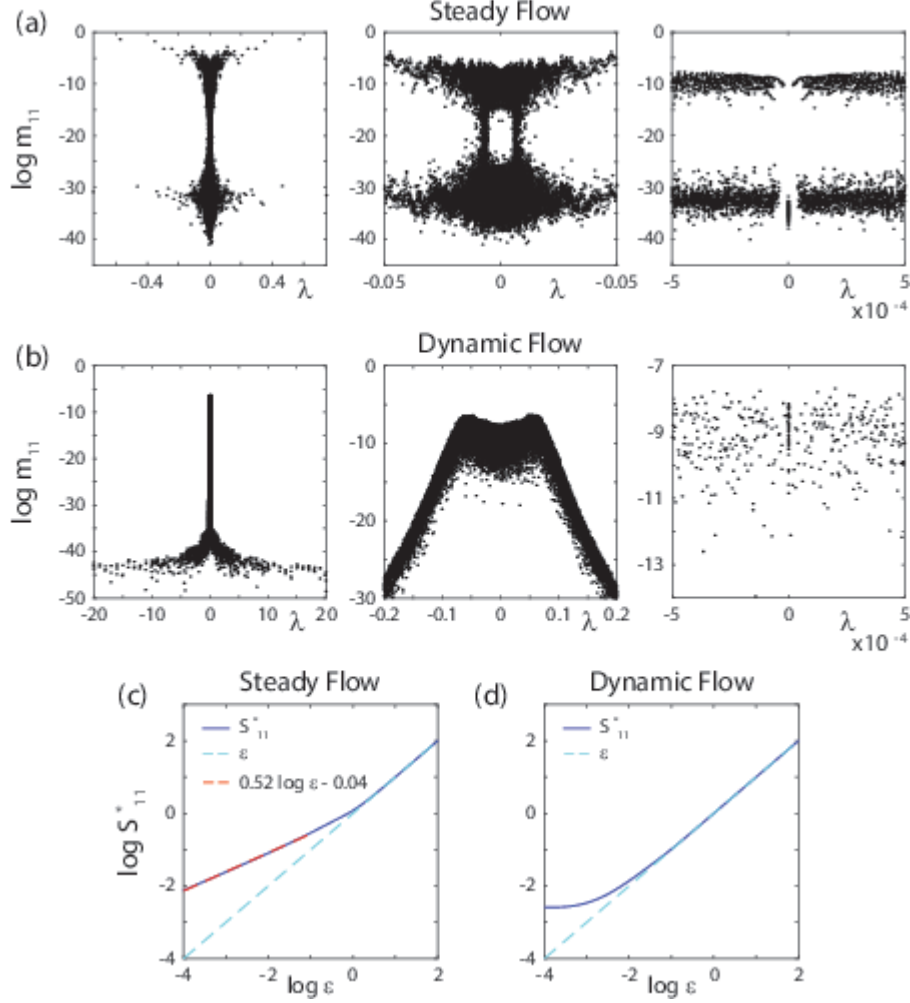


Figure 1: Computations of spectral measures and effective diffusivities for steady and dynamic flows. The spectral measure μ_{11} associated with the flow in (1) are displayed for (a) the steady setting and (b) the dynamic setting with the associated effective diffusivity S_{11}^* displayed in (c) and (d), respectively. In the steady case (a), the limit point of the measure near $\lambda = 0$ has small measure mass with $m_{11} \lesssim 10^{-30}$, leading to the asymptotic behavior $S_{11}^* \sim \epsilon^{1/2}$ for $\epsilon \ll 1$, displayed in (c). In the dynamic case (b), the significant measure mass $m_{11} \gtrsim 10^{-10}$ near $\lambda = 0$ leads to the asymptotic behavior $S_{11}^* \sim 1$ for $\epsilon \ll 1$, displayed in (d).