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

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

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

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

1. Introduction.

The long time, large scale motion of diffusing particles or tracers being advected by an incompressible flow field is equivalent to an enhanced diffusive process [86] 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 [44, 74, 19, 20, 18], turbulent combustion [3, 15, 85], and solute transport in porous media [12, 13, 90, 38, 45, 48, 46]. Time-dependent flows can have fluid velocity fields with chaotic dynamics, which gives rise to turbulence that greatly enhances the mixing, dispersion, and large scale transport of diffusing scalars.

In the climate system [24, 37], turbulence plays a key role in transporting mass, heat, momentum, energy, and salt in geophysical flows [61]. Turbulence enhances the dispersion of atmospheric gases [26] such as ozone [40, 71, 72, 73] and pollutants [23, 9, 78], as well as atmosphere-ocean transfers of carbon dioxide and other climatically important trace gas fluxes [92, 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 [91, 47, 16]. Chaotic motion of time-dependent fluid velocity fields cause instabilities in large scale ocean currents, generating geostrophic eddies [30] which dominate the kinetic energy of the ocean [31]. Geostrophic eddies greatly enhance [30] the meridional mixing of heat, carbon and other climatically important tracers, typically more than one order of magnitude greater than the mean flow of the ocean [81]. Eddies also impact heat and salt budgets through lateral fluxes and can extend the area of high biological productivity offshore by both eddy chlorophyll advection and eddy nutrient pumping [21]. In sea ice, which couples the atmosphere to the polar oceans [88], the transport of vast ice floes can also be enhanced by eddie fluxes [89, 50].

It has been noted in various geophysical contexts [72, 73] that eddy-induced, skew-diffusive tracer fluxes, directed normal to the tracer gradient [59], are generally equivalent to antisymmetric components in the effective diffusivity tensor D^*, while the symmetric part of D^* represents irreversible diffusive effects [75, 79, 36] directed down the tracer gradient. The mixing of eddy fluxes is typically non-divergent and unable to affect the evolution of the mean flow [59], and do not alter the tracer moments [36]. In this sense, the mixing is non-dissipative, reversible, and sometimes referred to as stirring [25, 36]. 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 [68]. This suggests that the effective diffusivity tensor D^* should be spatially and possibly also temporally inhomogeneous [68].

Due to the computational intensity of detailed climate models [37, 88, 64], 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 [49], atmospheric boundary layer turbulence [17], atmosphere-surface exchange over the sea [27] and sea ice [80, 1, 2, 87], and eddies in the ocean [55, 34]. 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 [65, 56, 8, 14, 28, 29, 54, 68, 70, 22, 39, 41, 52, 53]. Motivated by [66], it was shown [56] 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 [56]. 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 [56].

The incompressibility condition of the time-independent fluid velocity field was used [4, 5] to transform the cell problem in [56] into the quasi-static limit of Maxwell's equations [43, 35], which describe the transport properties of an electromagnetic wave in a composite material [60]. The analytic continuation method for representing transport in composites [35] provides Stieltjes integral representations for the bulk transport coefficients of composite media, such as electrical conductivity and permittivity, magnetic permeability, and thermal conductivity [60]. This method is based on the spectral theorem [84, 76] and a resolvent formula for, say, the electric field, involving a random self-adjoint operator [35, 63] or matrix [62]. Based on [35], 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* $\boldsymbol{\mu}$ 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 $\boldsymbol{\mu}$. This property led to rigorous bounds [5] for the diagonal components of D^*. Bounds for D^* can also be obtained using variational methods [5, 28, 29].

The mathematical framework developed in [56] was adapted [68, 57, 52] 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 [68] 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 [68]. This is consistent with what has been observed in geophysical flows in the climate system, as discussed above. In [57], this result was extended to weakly compressible, anelastic fluid velocity fields.

Based on [12], the cell problem discussed in [68] was transformed into a resolvent formula involving a self-adjoint operator, acting on the Sobolev space [58, 32] of spatially periodic scalar fields, which is also a Hilbert space. In the case where the mean flow and periodic fluctuations are time-independent, the self-adjoint operator is compact [12], hence *bounded* [82]. 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 [68] 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 [68] 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 $\boldsymbol{x} = (x, y)$,

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

The steady part $(\cos y, \cos x)$ of the flow is subject to a time-periodic perturbation that causes transition to Lagrangian chaos [14, 93]. 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, we present homogenization analysis and the integral representation formulas of the effective diffusion tensor in space-time periodic flows. In section 3, we discuss the Fourier method to compute spectral measure and effective diffusion. In Section **??**, we specialize the Fourier method to the fluid velocity field displayed in (1.1) and derive generalized eigenvalue problems for the spectral measure. In section Section **??**, we show numerical results that illustrate the difference of spectral measures and effective diffusivities in (1.1) when $\theta = 1$ and $\theta = 0$. Proofs of spectral representation formulas of effective diffusivity over vector and scalar fields as well as background materials are in the appendices.

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

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

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

We consider enhanced diffusive transport by a periodic fluid velocity field and non-dimensionalize equation (2.1) as follows. Let ℓ and T be typical length and time scales associated with the problem of interest. Mapping to the non-dimensional variables $t \mapsto t/T$ and $\boldsymbol{x} \mapsto \boldsymbol{x}/\ell$, one finds that ϕ satisfies the advection-diffusion equation in (2.1) with a non-dimensional molecular diffusivity $\varepsilon \mapsto T\,\varepsilon/\ell^2$ and velocity field $\boldsymbol{u} \mapsto T\,\boldsymbol{u}/\ell$. 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 [57, 52]. Here, we focus on the long time, large scale transport characteristics of equation (2.1) as a function of ε. To this end, we simply take T to be the temporal periodicity of the velocity field $\boldsymbol{u}$ and assume that the spatial periodicity of $\boldsymbol{u}$ is ℓ in all spatial dimensions, i.e.,

$$\boldsymbol{u}(t+T,\boldsymbol{x}) = \boldsymbol{u}(t,\boldsymbol{x}), \qquad \boldsymbol{u}(t,\boldsymbol{x}+\ell\,\boldsymbol{e}_j) = \boldsymbol{u}(t,\boldsymbol{x}), \quad j = 1,\ldots,d, \tag{2.2}$$

where $\boldsymbol{e}_j$ is a standard basis vector in the jth 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 [86] with an effective diffusivity tensor D^*. In recent decades, methods of homogenization theory [56, 28, 52] have been used to provide an explicit representation for D^*. In particular, these methods have demonstrated that the averaged or *homogenized* behavior of the advection-diffusion equation in (2.1), with space-time periodic velocity field $\boldsymbol{u}$, is determined by a diffusion equation involving an averaged scalar density $\bar{\phi}$ and an effective diffusivity tensor D^* [52]

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

Equation (2.3) follows from the assumption that the initial tracer density ϕ_0 varies slowly relative to the variations of the fluid velocity field $\boldsymbol{u}$ [56, 29, 52]. This information is incorporated into equation (2.1) by introducing a small dimensionless parameter $\delta \ll 1$ and writing [56, 29, 52]

$$\phi(0, \boldsymbol{x}) = \phi_0(\delta \boldsymbol{x}). \tag{2.4}$$

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

$$\boldsymbol{\xi} = \boldsymbol{x}/\delta, \quad \tau = t/\delta^\gamma, \qquad \gamma = 2. \tag{2.5}$$

The rescaled form of equation (2.1) is given by [52]

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

where we have denoted $\phi^\delta(t, \boldsymbol{x}) = \phi(t/\delta^2, \boldsymbol{x}/\delta)$. The convergence of ϕ^δ to $\bar{\phi}$ can be rigorously established in the following sense [52]

$$\lim_{\delta \to 0} \sup_{0 \le t \le t_0} \sup_{\boldsymbol{x} \in \mathbb{R}^d} |\phi^\delta(t, \boldsymbol{x}) - \bar{\phi}(t, \boldsymbol{x})| = 0, \tag{2.7}$$

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

For fixed $0 < \delta \ll 1$, an explicit representation of the effective diffusivity tensor D^* is given in terms of the (unique) mean zero, space-time periodic solution χ_j of the following *cell problem* [14, 52],

$$\partial_\tau \chi_j(\tau, \boldsymbol{\xi}) - \varepsilon \Delta_\xi \chi_j(\tau, \boldsymbol{\xi}) - \boldsymbol{u}(\tau, \boldsymbol{\xi}) \cdot \boldsymbol{\nabla}_\xi \chi_j(\tau, \boldsymbol{\xi}) = u_j(\tau, \boldsymbol{\xi}), \tag{2.8}$$

where the subscript ξ in Δ_ξ and $\boldsymbol{\nabla}_\xi$ indicates that differentiation is with respect to the fast variable $\boldsymbol{\xi}$ defined in equation (2.5). Specifically, the components D^*_{jk}, $j, k = 1, \dots, d$, of the matrix D^* are given by [56, 28, 52]

$$\mathsf{D}^*_{jk} = \varepsilon \delta_{jk} + \langle u_j \chi_k \rangle, \tag{2.9}$$

where δ_{jk} is the Kronecker delta and u_j is the jth component of the vector $\boldsymbol{u}$. The averaging $\langle \cdot \rangle$ in (2.9) is with respect to the fast variables defined in equation (2.5). More specifically, consider the bounded sets $\mathcal{T} \subset \mathbb{R}$ and $\mathcal{V} \subset \mathbb{R}^d$, with $\tau \in \mathcal{T}$ and $\boldsymbol{\xi} \in \mathcal{V}$, which define the space-time period cell ($(d+1)$–torus) $\mathcal{T} \times \mathcal{V}$. In the case of a time-dependent fluid velocity field, $\langle \cdot \rangle$ denotes space-time averaging over $\mathcal{T} \times \mathcal{V}$. In the special case of a time-independent fluid velocity field, the function χ_j is time-independent and satisfies equation (2.8) with $\partial_\tau \chi_j \equiv 0$, and $\langle \cdot \rangle$ in (2.9) denotes spatial averaging over $\mathcal{V}$ [28, 52]. Since the remainder of the analysis involves only the fast variables, for notational simplicity, we will drop the subscripts ξ displayed in equation (2.8).

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

$$\mathsf{D}^* = \mathsf{S}^* + \mathsf{A}^*, \qquad \mathsf{S}^* = \frac{1}{2}\left(\mathsf{D}^* + [\mathsf{D}^*]^T\right), \quad \mathsf{A}^* = \frac{1}{2}\left(\mathsf{D}^* - [\mathsf{D}^*]^T\right), \tag{2.10}$$

where $[\mathsf{D}^*]^T$ denotes transposition of the matrix D^*. Denote by S^*_{jk} and A^*_{jk}, $j, k = 1, \dots, d$, the components of S^* and A^* in (2.10). In Section C.1 we show that they have the following functional representations [68]

$$\mathsf{S}^*_{jk} = \varepsilon(\delta_{jk} + \langle \chi_j, \chi_k \rangle_1), \quad \mathsf{A}^*_{jk} = \langle A\chi_j, \chi_k \rangle_1, \qquad A = (-\Delta)^{-1}(\partial_\tau - \boldsymbol{u} \cdot \boldsymbol{\nabla}), \tag{2.11}$$

where $\langle f, h \rangle_1 = \langle \boldsymbol{\nabla} f \cdot \boldsymbol{\nabla} h \rangle$ is a Sobelov-type *sesquilinear* inner-product [58] and the operator $(-\Delta)^{-1}$ is based on convolution with respect to the Green's function for the Laplacian Δ [82]. 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 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 $\mathsf{A}^*_{kj} = \langle A\chi_k, \chi_j \rangle_1 = -\langle \chi_k, A\chi_j \rangle_1 = -\langle A\chi_j, \chi_k \rangle_1 = -\mathsf{A}^*_{jk}$ which, in turn, implies that A^* is an antisymmetric matrix, hence $\mathsf{A}^*_{kk} = \langle A\chi_k, \chi_k \rangle_1 = 0$.

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

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

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

$$\mathsf{S}^*_{jk} = \varepsilon\left(\delta_{jk} + \langle(\varepsilon + A)^{-1} g_j, (\varepsilon + A)^{-1} g_k\rangle_1\right), \quad \mathsf{A}^*_{jk} = \langle A(\varepsilon + A)^{-1} g_j, (\varepsilon + A)^{-1} g_k\rangle_1. \tag{2.13}$$

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 [84] $\lim_{\lambda\to\inf\Sigma} Q(\lambda) = 0$ and $\lim_{\lambda\to\sup\Sigma} Q(\lambda) = I$ [84], where I is the identity operator and Σ is the *spectrum* of M. Define the complex valued function $\mu_{jk}(\lambda) = \langle Q(\lambda) g_j, g_k\rangle_1$, $j, k = 1, \ldots, d$, where $g_j = (-\Delta)^{-1} u_j$ is defined in (2.12). Consider the positive measure μ_{kk} and the signed measures $\mathrm{Re}\,\mu_{jk}$ and $\mathrm{Im}\,\mu_{jk}$ associated with $\mu_{jk}(\lambda)$, introduced in equation (A.5). Then, given certain regularity conditions on the components u_j of the fluid velocity field $\boldsymbol{u}$, the functional formulas for S^*_{jk} and A^*_{jk} in (2.13) have the following Radon–Stieltjes integral representations, for all $0 < \varepsilon < \infty$ (see Section C.1 for details)

$$\mathsf{S}^*_{jk} = \varepsilon\left(\delta_{jk} + \int_{-\infty}^{\infty} \frac{\mathrm{dRe}\,\mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2}\right), \qquad \mathsf{A}^*_{jk} = -\int_{-\infty}^{\infty} \frac{\lambda\,\mathrm{dIm}\,\mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2}\,. \tag{2.14}$$

The periodic homogenization theorem summarized by equations (2.2)–(2.9), as well as its many variations [8, 65, 11, 13, 56, 5, 68, 69, 70, 57, 52], depend on the detailed nature of the fluid velocity field $\boldsymbol{u}$. They also depend on the temporal scaling used [13, 68, 52], i.e., what value of γ is used in equation (2.5). However, the mathematical structure of the cell problem in (2.8) and the functional form of D^* displayed in equation (2.9) remain unchanged for the space-time periodic setting. One of the key goals of the present work is to develop a rigorous mathematical framework that provides the Stieltjes integral representations for effective diffusivity tensor D^* displayed in (2.14), for space-time periodic $\boldsymbol{u}$. 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 (2.8) and the presence of an inner-product in the functional form of D^* in (2.9). In particular, the theoretical development is insensitive to the detailed nature of $\boldsymbol{u}$ and depends only on its boundedness properties (See Corollary C.2 for details). Consequently, our results given here apply in many of the well studied systems and will likely apply to many of the homogenization results of the future.

In order to illustrate the rich behaviors that can arise in the effective diffusivity tensor D^* for more general velocity fields and alternate temporal scalings, we now briefly discuss some key variations of the theory described above. When the fluid velocity field is mean-zero, as discussed above, then equation (2.7) holds and the effective diffusivity tensor D^* defined in (2.9) is constant [52]. Consequently, only the symmetric part of D^* plays a role in the effective transport equation displayed in (2.3). Now consider a more general fluid velocity field

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

which is the superposition of a *weak*, large-scale mean flow $\delta\boldsymbol{u}_0(\delta^2 t, \delta\boldsymbol{x})$ that varies on large spatial and slow time scales, with a mean-zero periodic flow $\boldsymbol{u}_1(t, \boldsymbol{x})$ that rapidly fluctuates in space and time [52]. If $\boldsymbol{u}_0(t, \boldsymbol{x})$ is smooth and bounded, the homogenization theorem for purely periodic velocity fields discussed above can be rigorously extended to the present setting and the effective transport equation in (2.3) is replaced by [52]

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

which includes an advective enhancement in transport by the large-scale mean flow $\boldsymbol{u}_0$ [52]. In this case, the effective diffusivity tensor D^* is completely independent of the mean flow $\boldsymbol{u}_0$, and is determined by the same formula in equation (2.9) and the same cell problem in (2.8) with $\boldsymbol{u} \to \boldsymbol{u}_1$ [52]. Consequently, D^* is again constant and only the symmetric part of D^* plays a role in the effective transport equation displayed in (2.16).

This problem was studied in [68] for scalings in (2.15) different than $\alpha = 1$ and $\gamma = 2$. The parameter α determines the strength of the mean flow $\boldsymbol{u}_0$ relative to the small scale periodic fluctuations $\boldsymbol{u}_1$. When the mean flow is weak compared to the fluctuations, to leading order, 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 D^* plays a role in the effective transport equation, which is similar to that in (2.16) [68]. Regardless of the values of α and γ, in the weak mean flow regime, the components D^*_{jk} of the effective diffusivity tensor are given by a formula analogous to equation (2.9) and the structure of the cell problem is analogous to equation (2.8). There are three distinct behaviors that arise as the values of α and γ vary, and the function χ_j in (2.8) can be time-dependent or time-independent ($\partial_\tau \chi_j \equiv 0$) [68].

As we discussed in Section 1, the constancy of the effective diffusivity tensor 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 D^* *is a function of space and time* [68]. Consequently, in the effective transport equation, the *antisymmetric* part of D^* contributes to a purely rotational (divergence-free) enhancement in advective transport, while the symmetric part of D^* contributes to an enhancement in advective and diffusive transport [68]. 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 (2.14), for both the symmetric and antisymmetric parts of the effective diffusivity tensor 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 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 $\boldsymbol{u}$, 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 D^* which lead to its promised integral representations. In Section D.1 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 D^* displayed in equations (2.14) and (D.14). For notational simplicity, we set $\boldsymbol{u} \to -\boldsymbol{u}$ and $(\tau, \boldsymbol{\xi}) \to (t, \boldsymbol{x})$ and write the operator A in (2.11) as $A = (-\Delta)^{-1}(\partial_t + \boldsymbol{u}\cdot\boldsymbol{\nabla})$. We will focus on the fluid velocity field $\boldsymbol{u}$ in equation (1.1), 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, densly defined subset of a Hilbert space $\mathscr{H}$ given in equation (C.3). Since the space-time periodic velocity field $\boldsymbol{u}$ in (1.1) is mean-zero, we require that the elements of $\mathscr{H}$ are also mean-zero, i.e., $f \in \mathscr{H}$ implies that $\langle f \rangle = 0$. In Section D.3 we discussed how a decomposition of the Hilbert space $\mathscr{H}$ provides a natural decomposition of the spectral measure μ_{jk} in (2.14) into its discrete and continuous components, as displayed in equation (D.10). Here, we demonstrate how this mathematical framework may be used to compute the discrete component of μ_{jk}, hence the discrete component of the Stieltjes integral representation for the effective diffusivity tensor D^* displayed in equation (D.14).

Rewrite the equation $A\varphi_n = \imath\lambda_n\varphi_n$ as

$$(\partial_t + \boldsymbol{u}\cdot\boldsymbol{\nabla})\varphi_n = -\imath\lambda_n\Delta\varphi_n. \tag{3.1}$$

For spatial dimension $d = 2$, the set of functions $\{\exp[\imath(\ell t + mx + ny)] \mid \ell, m, n \in \mathbb{Z}\}$ are complete in the

Hilbert space $\mathscr{H}$. Consequently, the eigenfunction $\varphi_l \in \mathscr{H}$ may be represented as

$$\varphi_l(t,\boldsymbol{x}) = \sum_\ell a^l_{\ell,m,n} \exp[\imath(\ell t + mx + ny)], \quad a^l_{\ell,m,n} = \langle \varphi_l, \exp(\imath(\ell t + mx + ny)\rangle_1, \tag{3.2}$$

where we have denoted $\boldsymbol{x} = (x, y)$. Write $\cos t = (\mathrm{e}^{\imath t} + \mathrm{e}^{-\imath t})/2$ and insert this and (3.2) into equation (3.1), yielding

$$\sum_\ell (\imath\ell + \boldsymbol{u}_1 \cdot \boldsymbol{\nabla} + \imath\lambda_n\Delta)\varphi^l_\ell(\boldsymbol{x})\mathrm{e}^{\imath\ell t} + \frac{\theta}{2}\sum_\ell (\mathrm{e}^{\imath(\ell+1)t} + \mathrm{e}^{\imath(\ell-1)t})\, \boldsymbol{u}_2 \cdot \boldsymbol{\nabla}\varphi^l_\ell(\boldsymbol{x}) = 0, \tag{3.3}$$

or:

$$\sum_\ell \left[(\imath\ell + \boldsymbol{u}_1 \cdot \boldsymbol{\nabla} + \imath\lambda_n\Delta)\varphi^l_\ell(\boldsymbol{x}) + \frac{\theta}{2}\boldsymbol{u}_2 \cdot \boldsymbol{\nabla}(\varphi^l_{\ell-1}(\boldsymbol{x}) + \varphi^l_{\ell+1}(\boldsymbol{x}))\right] \mathrm{e}^{\imath\ell t} = 0. \tag{3.4}$$

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

$$(\imath\ell + \boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi^l_\ell(\boldsymbol{x}) + \frac{\theta}{2}\boldsymbol{u}_2 \cdot \boldsymbol{\nabla}(\varphi^l_{\ell-1}(\boldsymbol{x}) + \varphi^l_{\ell+1}(\boldsymbol{x})) = -\imath\lambda_n\Delta\varphi^l_\ell(\boldsymbol{x}). \tag{3.5}$$

The system of partial differential equations in (3.5) can be reduced to a system of algebraic equations as follows. Recall that $\boldsymbol{u}_1(\boldsymbol{x}) = (\cos y, \cos x)$ and $\boldsymbol{u}_2(\boldsymbol{x}) = (\sin y, \sin x)$, which implies

$$\begin{aligned} (\boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi^l_\ell(\boldsymbol{x}) &= \cos y\, \partial_x\varphi^l_\ell(\boldsymbol{x}) + \cos x\, \partial_y\varphi^l_\ell(\boldsymbol{x}) \\ (\boldsymbol{u}_2 \cdot \boldsymbol{\nabla})\varphi^l_\ell(\boldsymbol{x}) &= \sin y\, \partial_x\varphi^l_\ell(\boldsymbol{x}) + \sin x\, \partial_y\varphi^l_\ell(\boldsymbol{x}) \end{aligned} \tag{3.6}$$

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

$$\varphi^l_\ell(\boldsymbol{x}) = \sum_{m,n} a^l_{\ell,m,n}\, \mathrm{e}^{\imath(mx+ny)} \tag{3.7}$$

Write $\cos x = (\mathrm{e}^{\imath x} + \mathrm{e}^{-\imath x})/2$ and $\sin x = (\mathrm{e}^{\imath x} - \mathrm{e}^{-\imath x})/(2\imath)$, for example, and insert this and (3.7) into equation (3.6), yielding

$$\begin{aligned} &(\boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi^l_\ell \\ &\qquad = \frac{1}{2}\sum_{m,n} a^l_{\ell,m,n}\left[\imath m\, \mathrm{e}^{\imath mx}(\mathrm{e}^{\imath(n+1)y} + \mathrm{e}^{\imath(n-1)y}) + \imath n\, \mathrm{e}^{\imath ny}(\mathrm{e}^{\imath(m+1)x} + \mathrm{e}^{\imath(m-1)x})\right] \\ &(\boldsymbol{u}_2 \cdot \boldsymbol{\nabla})\varphi^l_\ell \\ &\qquad = \frac{1}{2\imath}\sum_{m,n} a^l_{\ell,m,n}\left[\imath m\, \mathrm{e}^{\imath mx}(\mathrm{e}^{\imath(n+1)y} - \mathrm{e}^{\imath(n-1)y}) + \imath n\, \mathrm{e}^{\imath ny}(\mathrm{e}^{\imath(m+1)x} - \mathrm{e}^{\imath(m-1)x})\right] \end{aligned} \tag{3.8}$$

or:

$$\begin{aligned} (\boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi^l_\ell &= \frac{\imath}{2}\sum_{m,n}[m(a^l_{\ell,m,n-1} + a^l_{\ell,m,n+1}) + n(a^l_{\ell,m-1,n} + a^l_{\ell,m+1,n})]\mathrm{e}^{\imath(mx+ny)} \\ (\boldsymbol{u}_2 \cdot \boldsymbol{\nabla})\varphi^l_\ell &= \frac{1}{2}\sum_{m,n}[m(a^l_{\ell,m,n-1} - a^l_{\ell,m,n+1}) + n(a^l_{\ell,m-1,n} - a^l_{\ell,m+1,n})]\mathrm{e}^{\imath(mx+ny)}. \end{aligned} \tag{3.9}$$

We also have

$$-\Delta\varphi^l_\ell = \sum_{m,n} a^l_{\ell,m,n}(m^2 + n^2)\mathrm{e}^{\imath(mx+ny)} \tag{3.10}$$

By the completeness of the orthogonal set $\{e^{\imath(mx+ny)}\}$, inserting equations (3.9) and (3.10) into equation (3.5) yields

$$
\begin{aligned}
\imath\ell\, a^l_{\ell,m,n} &+ \frac{\imath}{2}[m(a^l_{\ell,m,n-1}+a^l_{\ell,m,n+1})+n(a^l_{\ell,m-1,n}+a^l_{\ell,m+1,n})] \\
&+\frac{\theta}{4}[m(a^l_{\ell-1,m,n-1}-a^l_{\ell-1,m,n+1})+n(a^l_{\ell-1,m-1,n}-a^l_{\ell-1,m+1,n}) \\
&\quad+m(a^l_{\ell+1,m,n-1}-a^l_{\ell+1,m,n+1})+n(a^l_{\ell+1,m-1,n}-a^l_{\ell+1,m+1,n})] \\
&=\imath\lambda_n(m^2+n^2)a^l_{\ell,m,n}, \qquad \ell,m,n\in\mathbb{Z},
\end{aligned} \tag{3.11}
$$

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

We now show that the special nature of the velocity field in (3.12) and the Fourier expansion of the eigenfunctions φ_n in (**??**) allow the spectral weights $\langle\varphi_n,g_j\rangle$ in equation (D.14) to be given in terms of the Fourier coefficients $a^l_{\ell,m,n}$ for the reduced index set $\ell,m,n\in\{-1,0,1\}$.

$$
\boldsymbol{u}(t,\boldsymbol{x})=(\cos y,\cos x)+\theta\cos t\,(\sin y,\sin x):=\boldsymbol{u}_1(\boldsymbol{x})+\theta\cos t\;\boldsymbol{u}_2(\boldsymbol{x}). \tag{3.12}
$$

Writing $\cos x=(e^{\imath x}+e^{-\imath x})/2$ and $\sin x=(e^{\imath x}-e^{-\imath x})/(2\imath)$, for example, from equation (3.12) we have that

$$
\begin{aligned}
u_1(t,x,y)&=\cos y+\theta\cos t\sin y \\
&=\frac{1}{2}\left(e^{\imath y}+e^{-\imath y}\right)+\frac{\theta}{4\imath}\left(e^{\imath t}+e^{-\imath t})(e^{\imath y}-e^{-\imath y}\right) \\
&=\frac{1}{2}\left(e^{\imath y}+e^{-\imath y}\right)+\frac{\theta}{4\imath}\left(e^{\imath(t+y)}-e^{\imath(t-y)}+e^{\imath(-t+y)}-e^{\imath(-t-y)}\right),
\end{aligned} \tag{3.13}
$$

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

$$
\begin{aligned}
\langle\varphi_n,g_1\rangle_1&=\frac{1}{2}\left(a^l_{0,0,1}+a^l_{0,0,-1}\right)+\frac{\theta}{4\imath}\left(a^l_{1,0,1}-a^l_{1,0,-1}+a^l_{-1,0,1}-a^l_{-1,0,-1}\right) \\
\langle\varphi_n,g_2\rangle_1&=\frac{1}{2}\left(a^l_{0,1,0}+a^l_{0,-1,0}\right)+\frac{\theta}{4\imath}\left(a^l_{1,1,0}-a^l_{1,-1,0}+a^l_{-1,1,0}-a^l_{-1,-1,0}\right)
\end{aligned} \tag{3.14}
$$

In the *time-independent case*, where $\theta=0$ in the velocity field of equation (3.12), the system of equations in (3.11) becomes

$$
m(a^l_{m,n-1}+a^l_{m,n+1})+n(a^l_{m-1,n}+a^l_{m+1,n})=2\lambda(m^2+n^2)a^l_{m,n}, \quad m,n\in\mathbb{Z}, \tag{3.15}
$$

while equation (3.14) becomes

$$
\langle\varphi_n,g_1\rangle_1=\frac{1}{2}\left(a^l_{0,1}+a^l_{0,-1}\right), \quad \langle\varphi_n,g_2\rangle_1=\frac{1}{2}\left(a^l_{1,0}+a^l_{-1,0}\right) \tag{3.16}
$$

where, for simplicity, we have dropped the super-script and sub-script, and have written $a_{m,n}=a^l_{m,n}$ and $\lambda=\lambda_n$.

4. Numerical Results. In Section 3, we used Fourier methods to transform the eigenvalue problem $A\varphi_l=\imath\lambda_l\varphi_l$ for the operator A in (2.11), involving the fluid velocity field in (1.1), 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 S^* and anti-symmetric A^* parts of the effective diffusivity tensor D^*, displayed in equations (2.14) and (D.14).

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

$$
a^l_{\ell,m,n}=0 \quad \text{if} \quad \max(|\ell|,|m|,|n|)>M, \tag{4.1}
$$

the infinite systems of equations in (3.11) and (3.15) become finite sets of equations. Consider the fluid velocity field in (1.1) 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

$$\begin{aligned} \Theta_d(\ell,m,n) &= (M+m+1)+(M+n)(2M+1)+(M+\ell)(2M+1)^2, \\ \Theta_s(m,n) &= (M+m+1)+(M+n)(2M+1), \end{aligned} \tag{4.2}$$

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

$$\mathsf{B}\boldsymbol{a}_l = \lambda_l \mathsf{C}\boldsymbol{a}_l. \tag{4.3}$$

Here B is a symmetric matrix and 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, B is Hermitian in the dynamic case and is real-symmetric in the steady case, while the matrix C is real-symmetric and diagonal in both cases. Since B and C are symmetric matrices, the generalized eigenvalues λ_l are real-valued and the eigen-vectors $\boldsymbol{a}_l$ – consisting of the Fourier coefficients for φ_l – satisfy the orthogonality condition [67]

$$\boldsymbol{a}_j^\dagger \mathsf{C}\boldsymbol{a}_k = \delta_{jk}. \tag{4.4}$$

The matrix C is positive semidefinite and diagonal. However, in the steady case, in both of the matrices B and C, the row and column associated with the Fourier coefficient $a^l_{0,0}$ is all zeros, as can be seen from equation (3.15). Since the eigenfunction φ_l is mean-zero, we have that $a^l_{0,0} = 0$. Therefore, we simply remove this row and column in both B and C so that C becomes strictly positive definite.

In the dynamic case, the entries of the matrix C do not depend on ℓ. Consequently, we have that $\mathsf{C} = \operatorname{diag}(\mathsf{C}_s,\dots,\mathsf{C}_s)$, where we have denoted by C_s the matrix C in the steady case. Therefore, there are $2M+1$ diagonal entries in C with the value zero, corresponding to $m = n = 0$. The entries of the corresponding rows and columns of the matrix B are all zero except for the diagonal entry, which has the value ℓ, as can be seen from equation (3.11). This implies that $\ell a^l_{\ell,0,0} = 0$ for all $-M \le \ell \le M$. Since the eigenfunction φ_l is mean-zero in time *and* space, we have that $a^l_{\ell,0,0} = 0$ for all $-M \le \ell \le M$, which is consistent with the above observation. We therefore simply remove the corresponding rows and columns in both B and C so that C becomes strictly positive definite. This method of removing the null space common to both B and C is called *deflation* [67].

Now that the matrix C is strictly positive definite and diagonal, the matrix C^q is well defined for all $q \in \mathbb{R}$, with entries $(\mathsf{C}^q)_{ij} = \mathsf{C}^q_{ii}\delta_{ij}$, where C^q_{ii} is the ith diagonal of the matrix C raised to the power q, and $\mathsf{C}^q\mathsf{C}^{-q} = \mathsf{I}$. Consequently, the generalized eigenvalue problem in equation (4.3) can be written as the following standard eigenvalue problem

$$\mathsf{C}^{-1/2}\mathsf{B}\mathsf{C}^{-1/2}\boldsymbol{v}_l = \lambda_l \boldsymbol{v}_l, \qquad \boldsymbol{v}_l = \mathsf{C}^{1/2}\boldsymbol{a}_l. \tag{4.5}$$

Since B is a symmetric matrix and C is diagonal, the matrix $\mathsf{C}^{-1/2}\mathsf{B}\mathsf{C}^{-1/2}$ is also symmetric with real-valued eigenvalues and orthonormal eigenvectors. From the orthogonality relation $\boldsymbol{v}_j^\dagger \boldsymbol{v}_k = \delta_{jk}$ we recover equation (4.4) via $\boldsymbol{v}_l = \mathsf{C}^{1/2}\boldsymbol{a}_l$ in (4.5).

In summary, our numerical method is the following. Create the matrices B and C according to equation (3.11) or (3.15) and the corresponding bijective mapping in (4.2). Remove the rows and columns of the matrices B and C corresponding to $\mathsf{C}_{ii} = 0$. Compute the eigenvalues λ_l and eigenvectors $\boldsymbol{v}_l$ of the symmetric matrix $\mathsf{C}^{-1/2}\mathsf{B}\mathsf{C}^{-1/2}$. The computed Fourier coefficients of the eigenfunction φ_l are given by $\boldsymbol{a}_l = \mathsf{C}^{-1/2}\boldsymbol{v}_l$. The eigenvalues associated with the discrete component of the spectral measure displayed in equation (D.14) are given by λ_l, while the spectral measure weights $\langle \varphi_n, g_1\rangle_1$ and $\langle \varphi_n, g_2\rangle_1$ in (D.14) are determined by the vector $\boldsymbol{a}_l$ via equation (3.14) or (3.16).

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 $\mathsf{C}^{-1/2}\mathsf{B}\mathsf{C}^{-1/2}$ 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.

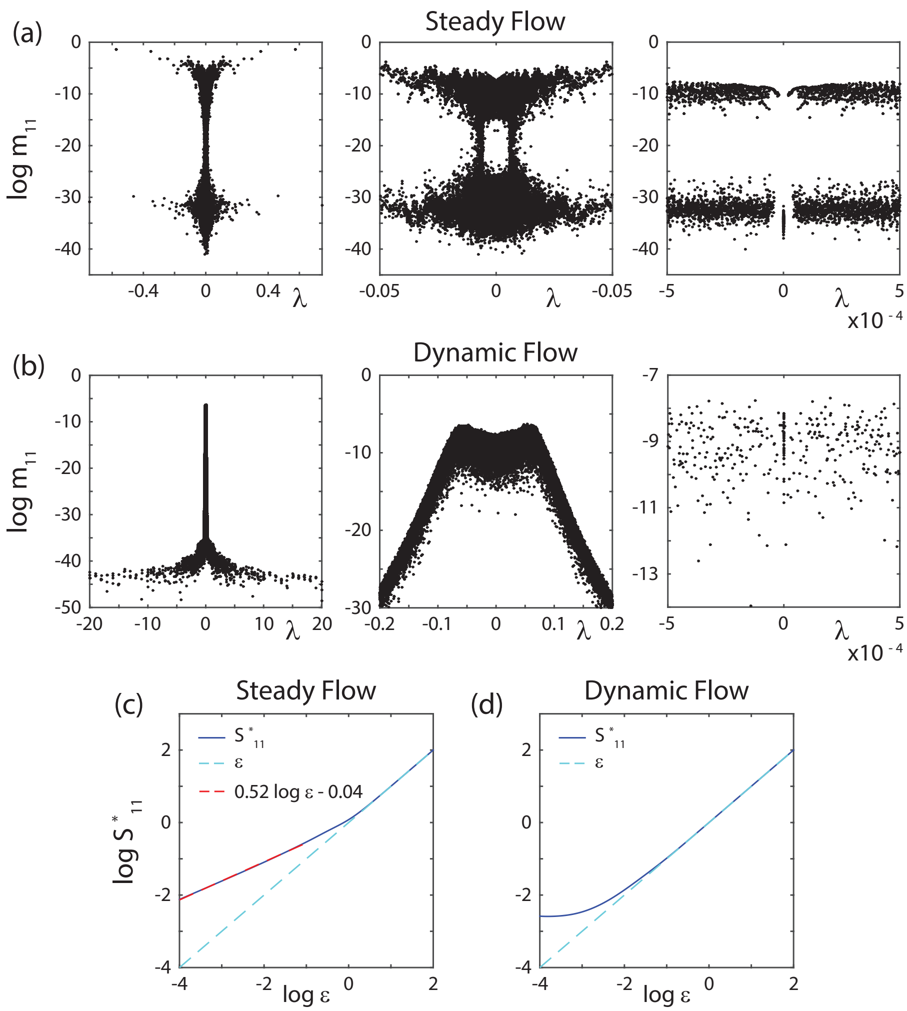

FIG. 1. *Computations of spectral measures and effective diffusivities for steady and dynamic flows. The spectral measure* μ_{11} *associated with the flow in* (1.1) *are displayed for (a) the steady setting and (b) the dynamic setting with the associated effective diffusivity* S^*_{11} *displayed in (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* $\mathsf{S}^*_{11} \sim \varepsilon^{1/2}$ *for* $\varepsilon \ll 1$*, 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* $\mathsf{S}^*_{11} \sim 1$ *for* $\varepsilon \ll 1$*, displayed in (d).*

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 $\boldsymbol{u}$ displayed in equation (1.1), for (a) the steady ($\theta = 0$) and (b) the dynamic ($\theta = 1$) settings. Here, the spectral weights $m_{11}(l) = |\langle \varphi_l, g_1 \rangle_1|^2$ are determined by equations (3.16) and (3.14), respectively. Consistent with the symmetries of the flows [14], we have $\mu_{11} = \mu_{22}$, while $\mathrm{Re}\,\mu_{12} = 0$ and $\mathrm{Im}\,\mu_{12} = 0$, up to numerical accuracy and finite size effects. For the 2D steady cell flow in (1.1) with $\theta = 0$, it is known [28] that $\mathsf{S}^*_{11} \sim \varepsilon^{1/2}$ 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 $(-\Delta)^{-1}[\boldsymbol{u}_1 \cdot \boldsymbol{\nabla}]$ is compact [12] and therefore has bounded, discrete spectrum away from the spectral origin, with a limit point at $\lambda = 0$ [82]. 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 [28] $\mathsf{S}^*_{11} \sim \varepsilon^{1/2}$ as $\varepsilon \to 0$ demonstrates that the spectral measure μ_{11} of the operator $(-\Delta)^{-1}[\boldsymbol{u}_1 \cdot \boldsymbol{\nabla}]$ 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 (1.1), 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, $\mathsf{S}^*_{11} \sim 1$ for $\varepsilon \ll 1$, as shown in Fig. 1(d). This is consistent with numerical computations of S^*_{11} using alternate methods [14], showing that S^*_{11} plateaus off at ≈ 1.5. The discrepancy between our result and that in [14] 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 a part of current 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 [76, 84].

Let Φ be a linear operator acting on a Hilbert space $\mathscr{H}$ with sesquilinear inner-product $\langle\cdot,\cdot\rangle$ satisfying $\langle a\psi, b\varphi\rangle = a\,\overline{b}\,\langle\psi,\varphi\rangle$ and $\langle\psi,\varphi\rangle = \overline{\langle\varphi,\psi\rangle}$ for all $\psi,\varphi \in \mathscr{H}$ and $a, b \in \mathbb{C}$, where $\overline{z}$ denotes complex conjugation of $z \in \mathbb{C}$. The $\mathscr{H}$–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., $\|\Phi\| = \sup_{\{\psi\in\mathscr{H}\,:\,\|\psi\|=1\}}\|\Phi\psi\| < \infty$, then $\|\Phi^*\| = \|\Phi\|$ [76]. Consequently, Φ and its adjoint Φ^* have identical domains,

$$D(\Phi) = D(\Phi^*), \tag{A.1}$$

as they can be taken, without loss of generality [82], to be the entire Hilbert space, $D(\Phi) = D(\Phi^*) = \mathscr{H}$. The operator Φ is said to be *symmetric* if [76]

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

By definition [76, 84], the two properties (A.1) and (A.2) together imply that the operator Φ is *self-adjoint*, i.e. $\Phi \equiv \Phi^*$ on $D(\Phi)$.

Conversely, the Hellinger–Toeplitz theorem states, if the operator Φ satisfies $\langle\Phi\psi,\varphi\rangle = \langle\psi,\Phi\varphi\rangle$ for *every* $\psi,\varphi \in \mathscr{H}$, then Φ is bounded on $\mathscr{H}$ [76]. This suggests that, if Φ is *unbounded* on $\mathscr{H}$, then it is defined as a self-adjoint operator only on a proper subset of $\mathscr{H}$. However, the domain $D(\Phi)$ can sometimes be defined as an *everywhere dense* subset of $\mathscr{H}$ such that Φ is bounded. On this domain, the symmetric operator Φ can be extended to a *closed* symmetric operator [76, 84]. 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 [84]. Only for self-adjoint operators does the spectral theorem hold [76, 84].

The spectrum Σ of a self-adjoint operator Φ on a Hilbert space $\mathscr{H}$ is real-valued [76, 84]. If Φ is bounded, then its spectral radius equal to its operator norm $\|\Phi\|$ [76], i.e.,

$$\Sigma \subseteq [-\|\Phi\|, \|\Phi\|\,]. \tag{A.3}$$

If Φ is unbounded, its spectrum Σ can be an unbounded subset of, or can even coincide with the set of real numbers $\mathbb{R}$ [84].

We now summarize the spectral theorem for self-adjoint operators [84]. Let Φ be a self-adjoint operator with densely defined domain $D(\Phi) \subset \mathscr{H}$. If Φ is bounded then we simply take $D(\Phi) \equiv \mathscr{H}$. 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 [84]

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

where 0 and I denote the null and identity operators on $\mathscr{H}$, 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 $\psi,\varphi \in D(\Phi)$ [84].

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

$$\operatorname{Re}\mu_{\psi\varphi}(\lambda) = \frac{1}{2}\left(\mu_{\psi\varphi}(\lambda) + \overline{\mu}_{\psi\varphi}(\lambda)\right), \quad \operatorname{Im}\mu_{\psi\varphi}(\lambda) = \frac{1}{2\imath}\left(\mu_{\psi\varphi}(\lambda) - \overline{\mu}_{\psi\varphi}(\lambda)\right), \tag{A.5}$$

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 [83, 84, 33]

$$\begin{aligned} \mathrm{d}\mu_{\psi\varphi}(\lambda) &= \mathrm{d}\langle Q(\lambda)\psi, \varphi\rangle, & \mathrm{dRe}\,\mu_{\psi\varphi}(\lambda) &= \mathrm{dRe}\,\langle Q(\lambda)\psi, \varphi\rangle, \\ \mathrm{d}\mu_{\psi\psi}(\lambda) &= \mathrm{d}\|Q(\lambda)\psi\,\|^2, & \mathrm{dIm}\,\mu_{\psi\varphi}(\lambda) &= \mathrm{dIm}\,\langle Q(\lambda)\psi, \varphi\rangle, \end{aligned} \tag{A.6}$$

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 [83, 84].

The spectral theorem also provides an operational calculus in Hilbert space which yields powerful integral representations involving the Stieltjes measures displayed in equation (A.6). A summary of the relevant details are as follows. Let $F(\lambda)$ and $G(\lambda)$ be arbitrary complex-valued functions and denote by $\mathscr{D}(F)$ 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 $\mathscr{D}(G)$. Then $\mathscr{D}(F)$ and $\mathscr{D}(G)$ are linear manifolds and there exists linear operators denoted by $F(\Phi)$ and $G(\Phi)$ with domains $\mathscr{D}(F)$ and $\mathscr{D}(G)$, respectively, which are defined in terms of the following Radon–Stieltjes integrals [84]

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

where the integration in (A.7) is over the spectrum Σ of Φ [76, 84].

The mass $\mu^0_{\psi\varphi} = \int_{-\infty}^{\infty}\mathrm{d}\mu_{\psi\varphi}(\lambda)$ of the Stieltjes measure $\mu_{\psi\varphi}$ satisfies [84] $\mu^0_{\psi\varphi} = \lim_{\lambda\to\sup\Sigma}\mu_{\psi\varphi}(\lambda) - \lim_{\lambda\to\inf\Sigma}\mu_{\psi\varphi}(\lambda)$. Consequently, equation (A.4) yields

$$\mu^0_{\psi\varphi} = \int_{-\infty}^{\infty}\mathrm{d}\langle Q(\lambda)\psi, \varphi\,\rangle = \langle\psi, \varphi\rangle, \qquad |\mu^0_{\psi\varphi}| \leq \|\psi\|\,\|\varphi\| < \infty. \tag{A.8}$$

Equation (A.8) demonstrates that the measures in (A.6) are *finite measures*, i.e., they have bounded mass [84].

Equation (A.7) can be generalized, holding with suitable notational changes, for *maximal normal operators* [84]. Such a normal operator $\mathbf{N}$ with densely defined domain $D(\mathbf{N}) \subset \mathscr{H}$ 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 $\mathbb{C}$ [84]. 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 [84]. 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 $\operatorname{Re}\mu_{\psi\varphi}$ and $\operatorname{Im}\mu_{\psi\varphi}$ displayed in equation (A.6) 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,

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

Now consider the special cases $F(\mathbf{N}) = G(\mathbf{N})$ and $F(\mathbf{N}) = \mathbf{N}G(\mathbf{N})$, i.e., $F(\imath\lambda) = G(\imath\lambda)$ and $F(\imath\lambda) = \imath\lambda G(\imath\lambda)$ in equation (A.7), respectively. It follows from equations (A.7) and (A.9), the identities $\operatorname{Re} z = (z + \overline{z})/2$

and $\mathrm{Im}\, z = (z - \overline{z})/(2\imath)$, and the linearity properties [84] of Stieltjes-Radon integrals with respect to the functions $\mu_{\psi\varphi}(\lambda)$ and $\overline{\mu}_{\psi\varphi}(\lambda)$ that

$$\text{(A.10)} \qquad \begin{aligned} \langle G(\mathbf{N})\psi, G(\mathbf{N})\varphi\rangle &= \int_{-\infty}^{\infty} |G(\imath\lambda)|^2 \, \mathrm{dRe}\, \mu_{\psi\varphi}(\lambda), \\ \langle \mathbf{N}G(\mathbf{N})\psi, G(\mathbf{N})\varphi\rangle &= -\int_{-\infty}^{\infty} \lambda\, |G(\imath\lambda)|^2 \, \mathrm{dIm}\, \mu_{\psi\varphi}(\lambda). \end{aligned}$$

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 $\psi \in \mathscr{H}$ such that the Stieltjes integral $\int_{-\infty}^{\infty} \lambda^2 \, \mathrm{d}\mu_{\psi\psi}(\lambda)$ is convergent. When $\psi \in D(\Phi)$ the element $\Phi\psi$ is determined by the relations [84]

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

where φ is an arbitrary element in $D(\Phi)$ [84]. In fact, this determines the one-to-one correspondence between the self-adjoint operator Φ and its resolution of the identity $Q(\lambda)$ [84].

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

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

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 $n \to \infty$. 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 $-\imath\partial_t$ 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 $-\imath\partial_t$ is a bounded linear self-adjoint operator [76, 84]. Consider the class $\mathscr{A}_\mathcal{T}$ of all functions $\psi \in L^2(\mathcal{T})$ such that $\psi(t)$ is *absolutely continuous* [77] on the interval $\mathcal{T}$ and has a derivative $\psi'(t)$ belonging to $L^2(\mathcal{T})$, i.e., [84, 77]

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

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

$$\text{(B.3)} \qquad \tilde{\mathscr{A}_\mathcal{T}} = \{\psi \in \mathscr{A}_\mathcal{T} \,|\, \psi(0) = \psi(T)\}, \qquad \hat{\mathscr{A}_\mathcal{T}} = \{\psi \in \mathscr{A}_\mathcal{T} \,|\, \psi(0) = \psi(T) = 0\}.$$

These function spaces satisfy $\hat{\mathscr{A}_\mathcal{T}} \subset \tilde{\mathscr{A}_\mathcal{T}} \subset \mathscr{A}_\mathcal{T}$ and are each everywhere dense in $L^2(\mathcal{T})$ [84]. Let the operators B, $\tilde{B}$, and $\hat{B}$ be identified as $-\imath\partial_t$ with domains $\mathscr{A}_\mathcal{T}$, $\tilde{\mathscr{A}_\mathcal{T}}$, and $\hat{\mathscr{A}_\mathcal{T}}$, 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 $\hat{B}$ [84]. In symbols, this means that $\tilde{B} = \tilde{B}^*$ on $\tilde{\mathscr{A}_\mathcal{T}}$ and $D(\tilde{B}) = D(\tilde{B}^*) = \tilde{\mathscr{A}_\mathcal{T}}$, i.e., $\tilde{B} \equiv \tilde{B}^*$ on $\tilde{\mathscr{A}_\mathcal{T}}$. This establishes that the operator $-\imath\partial_t$ with domain $\tilde{\mathscr{A}_\mathcal{T}}$ is self-adjoint, hence ∂_t is a maximal skew-symmetric (normal) operator on $\tilde{\mathscr{A}_\mathcal{T}}$. The operator $\imath\partial_t$ on $\tilde{\mathscr{A}_\mathcal{T}}$ has a simple point spectrum, consisting of eigenvalues $\lambda = 2n\pi/T$, $n \in \mathbb{Z}$, with corresponding eigenfunctions $\exp(2n\pi t/T)$ [84].

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 [68], while in Section C.2 we 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.1 we use the one-to-one correspondence between a self-adjoint operator and its resolution of the identity [84], discussed in the paragraph containing equation (A.11), to establish that the two approaches are equivalent.

C.1. Scalar fields and the effective diffusivity. In this section we provide an abstract Hilbert space formulation of the effective parameter problem for advection enhanced diffusion by a space-time periodic fluid velocity field $\boldsymbol{u}(t,\boldsymbol{x})$. 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 $\boldsymbol{u}(t,\boldsymbol{x})$. 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 $\mathscr{H}_\mathcal{T}$ and $\mathscr{H}_\mathcal{V}$,

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

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

In equation (B.3) we defined the space $\tilde{\mathscr{A}_\mathcal{T}}$ of absolutely continuous $\mathcal{T}$-periodic functions with derivatives belonging to $\mathscr{H}_\mathcal{T}$, which is an everywhere dense subset of the Hilbert space $\mathscr{H}_\mathcal{T}$ [84]. We now define the Sobolev space $\mathscr{H}_\mathcal{V}^1$, which is also a Hilbert space [12, 32, 58],

$$\mathscr{H}_\mathcal{V}^1=\big\{\psi\in\mathscr{H}_\mathcal{V}\ |\ \langle|\boldsymbol{\nabla}\psi|^2\rangle_\mathcal{V}<\infty\big\}, \tag{C.2}$$

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

$$\mathscr{H}=\mathscr{H}_\mathcal{T}\otimes\mathscr{H}_\mathcal{V}^1,\qquad \mathscr{F}=\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}_\mathcal{V}^1. \tag{C.3}$$

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

We now use properties of the Hilbert space $\mathscr{H}$ to obtain functional formulas for the symmetric S^* and antisymmetric A^* parts of the effective diffusivity tensor D^* defined in equations (2.9) and (2.10), involving the solution χ_j of the cell problem in equation (2.8) and a maximal skew-symmetric operator A on $\mathscr{F}$. 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 S^* and A^*. We will henceforth assume that $u_j,\chi_j\in\mathscr{F}$ for all $j=1,\dots,d$.

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

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

where we have defined $A=(-\Delta)^{-1}(\partial_t-\boldsymbol{u}\cdot\boldsymbol{\nabla})$. The operator $(-\Delta)^{-1}$ is based on convolution with respect to the Green's function for the Laplacian Δ and is bounded on $L^2(\mathcal{V})$ [82], hence $\mathscr{H}_\mathcal{V}^1$. Now write the functional $\langle u_j\chi_k\rangle$ in equation (2.9) as [68]

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

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

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

Proof of Theorem C.1. We first establish that $M=-\imath A$ is a self-adjoint operator on $\mathscr{F}$. The Sobelov space $\mathscr{H}^1_{\mathcal{V}}$ in (C.2) is the closure in the norm $\langle|\boldsymbol{\nabla}\psi|^2\rangle_{\mathcal{V}}$ of the space of all twice continuously differentiable periodic functions in $\mathscr{H}_{\mathcal{V}}$, and all the elements of $\mathscr{H}^1_{\mathcal{V}}$ are those elements of $\mathscr{H}_{\mathcal{V}}$ which have square integrable gradients on the set $\mathcal{V}$ [12]. Furthermore, the elements of $\tilde{\mathscr{A}_{\mathcal{T}}}$ are those elements of $\mathscr{H}_{\mathcal{T}}$ 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 [77]. Consequently, $f\in\mathscr{F}$ implies that [84, 77]

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

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

We have already established in Section B that the operator $-\imath\partial_t$ with domain $\tilde{\mathscr{A}_{\mathcal{T}}}$ is self-adjoint [84]. The integral operator $(-\Delta)^{-1}$ is self-adjoint and compact on $\mathscr{H}_{\mathcal{V}}$ [82]. Since they commute on $\tilde{\mathscr{A}_{\mathcal{T}}}\otimes\mathscr{H}_{\mathcal{V}}$ [33], it follows that the operator $-\imath(-\Delta)^{-1}\partial_t$ is self-adjoint with domain $\tilde{\mathscr{A}_{\mathcal{T}}}\otimes\mathscr{H}_{\mathcal{V}}$, hence $(-\Delta)^{-1}\partial_t$ is a maximal (skew-symmetric) normal operator on the same domain [84].

We now establish that the operator $(-\Delta)^{-1}[\boldsymbol{u}\cdot\boldsymbol{\nabla}]$ is antisymmetric and compact on $\mathscr{F}$. The antisymmetry of this operator depends on the incompressibility, $\boldsymbol{\nabla}\cdot\boldsymbol{u}=0$, of the fluid velocity field and was established in [12, 68]. Since the operator $(-\Delta)^{-1}$ is compact on $\mathscr{H}_{\mathcal{V}}$ [82], we need only show that the operator $\boldsymbol{u}\cdot\boldsymbol{\nabla}$ is bounded on $\mathscr{F}$. This is established by the following calculation. For $u_j,f\in\mathscr{F}$, equation (C.6) yields

$$\begin{aligned}
\|\boldsymbol{u}\cdot\boldsymbol{\nabla}f\|^2&=|\langle\boldsymbol{u}\cdot\boldsymbol{\nabla}f,\boldsymbol{u}\cdot\boldsymbol{\nabla}f\rangle|\\
&\le\sum_{jk}|\langle u_j\partial_jf,u_k\partial_kf\rangle|\quad\text{(triangle inequality)}\\
&\le\max_j\|u_j\|^2_\infty\sum_{jk}|\langle\partial_jf,\partial_kf\rangle|\\
&\le\max_j\|u_j\|^2_\infty\sum_{jk}\|\partial_jf\|\,\|\partial_kf\|\quad\text{(Cauchy-Schwartz)}\\
&=\max_j\|u_j\|^2_\infty\Big[\sum_j\|\partial_jf\|\Big]^2\\
&\le d\,\max_j\|u_j\|^2_\infty\sum_j\|\partial_jf\|^2\quad\text{(Cauchy-Schwartz)}\\
&=d\,\max_j\|u_j\|^2_\infty\,\|f\|^2_1.
\end{aligned} \tag{C.7}$$

This demonstrates that the operator norm $\|\boldsymbol{u}\cdot\boldsymbol{\nabla}\|$ has the upper bounded $\|\boldsymbol{u}\cdot\boldsymbol{\nabla}\|\le\sqrt{d}\,\max_j\|u_j\|_\infty<\infty$ and establishes that $(-\Delta)^{-1}[\boldsymbol{u}\cdot\boldsymbol{\nabla}]$ is a compact operator on $\mathscr{F}$. Since $(-\Delta)^{-1}[\boldsymbol{u}\cdot\boldsymbol{\nabla}]$ is antisymmetric and bounded on $\mathscr{F}$, it is a maximal (skew-adjoint) normal operator on $\mathscr{F}$, hence $-\imath(-\Delta)^{-1}[\boldsymbol{u}\cdot\boldsymbol{\nabla}]$ is self-adjoint on $\mathscr{F}$ [84].

Denote $M=-\imath A$, where $A=(-\Delta)^{-1}(\partial_t-\boldsymbol{u}\cdot\boldsymbol{\nabla})$. Since $-\imath(-\Delta)^{-1}[\boldsymbol{u}\cdot\boldsymbol{\nabla}]$ is a self-adjoint operator with domain containing $\mathscr{F}$ and $-\imath(-\Delta)^{-1}\partial_t$ is self-adjoint with domain $\tilde{\mathscr{A}_{\mathcal{T}}}\otimes\mathscr{H}_{\mathcal{V}}$, the operator M is self-adjoint with domain $D(M)\supset(\tilde{\mathscr{A}_{\mathcal{T}}}\otimes\mathscr{H}_{\mathcal{V}})\cap\mathscr{F}=\mathscr{F}$ [84].

The complex-valued functions involved in the functional formulas for S^*_{jk} and A^*_{jk} in equation (2.13) are $F(\lambda)=(\varepsilon+\imath\lambda)^{-1}$ and $G(\lambda)=\imath\lambda(\varepsilon+\imath\lambda)^{-1}$. For all $0<\varepsilon<\infty$, we have $|F(\lambda)|^2=(\varepsilon^2+\lambda^2)^{-1}\le\varepsilon^{-2}<\infty$ and $|G(\lambda)|^2=\lambda^2(\varepsilon^2+\lambda^2)^{-1}\le1$. Since μ_{kk} is a finite measure for all $k=1,\dots,d$, as shown in equation (A.8), we therefore have that $f \in \mathscr{D}(F)$ and $f \in \mathscr{D}(G)$ for all $f \in D(M)$ when $0 < \varepsilon < \infty$. Since $u_j \in \mathscr{F}$ and $(-\Delta)^{-1}$ is a bounded operator on $\mathscr{F}$, we have that $g_j = (-\Delta)^{-1} u_j \in \mathscr{F}$. We note that in the mean-zero setting, $\langle u_j \rangle = 0$ and the Fubini-Tonelli theorem [33] 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 (A.7) hold for the functions $F(\lambda)$ and $G(\lambda)$ defined above, involving the complex measure μ_{jk}. The discussion leading to equation (A.10) then establishes the integral representations for S^*_{jk} and A^*_{jk} displayed in equation (2.14). This completes the proof of Theorem C.1 □.

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

Corollary C.2. *Theorem C.1 can be extended to the following class $\mathscr{U}$ of fluid velocity fields $\boldsymbol{u}$, having components u_j, $j = 1, \ldots, d$,*

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

Corollary C.2 states that the requirement $u_j \in \mathscr{F} = \tilde{\mathscr{A}}_{\mathcal{T}} \otimes \mathscr{H}^1_{\mathcal{V}}$ can be weakened to $u_j \in \tilde{\mathscr{A}}_{\mathcal{T}} \otimes \mathscr{H}_{\mathcal{V}}$ such that the operator $(-\Delta)^{-1}[\boldsymbol{u} \cdot \boldsymbol{\nabla}]$ is bounded on $\mathscr{F}$. The set $\mathscr{U}$ in (C.8) is non-empty. We established this in (C.7), showing that $\{u_j \in \tilde{\mathscr{A}}_{\mathcal{T}} \otimes \mathscr{H}_{\mathcal{V}} \mid \|u_j\|_\infty < \infty\} \subset \mathscr{U}$, as $(-\Delta)^{-1}$ is a bounded operator on $\mathscr{H}_{\mathcal{V}}$ [82]. This extension of Theorem C.1 allows for spatially *unbounded flows* with square integrable singularities.

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

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

$$\mathcal{H}_{\mathcal{T}} = \otimes_{j=1}^d \mathscr{H}_{\mathcal{T}}, \qquad \mathcal{H}_{\mathcal{V}} = \otimes_{j=1}^d \mathscr{H}_{\mathcal{V}}, \qquad \mathcal{F} = \otimes_{j=1}^d \mathscr{F}. \tag{C.9}$$

By the Helmholtz theorem [51, 10], the Hilbert space $\mathcal{H}_{\mathcal{V}}$ can be decomposed into mutually orthogonal subspaces of curl-free $\mathcal{H}_\times$, divergence-free $\mathcal{H}_\bullet$, and constant $\mathcal{H}_0$ vector fields, with $\mathcal{H}_{\mathcal{V}} = \mathcal{H}_\times \oplus \mathcal{H}_\bullet \oplus \mathcal{H}_0$. The orthogonal projectors associated with this decomposition are given by $\boldsymbol{\Gamma}_\times = -\boldsymbol{\nabla}(-\Delta)^{-1}\boldsymbol{\nabla}\boldsymbol{\cdot}$, $\boldsymbol{\Gamma}_\bullet = \boldsymbol{\nabla} \times (-\boldsymbol{\Delta})^{-1} \boldsymbol{\nabla} \times$, and $\boldsymbol{\Gamma}_0 = \langle \cdot \rangle$, respectively, satisfying $\mathsf{I} = \boldsymbol{\Gamma}_\times + \boldsymbol{\Gamma}_\bullet + \boldsymbol{\Gamma}_0$ [28, 60]. Here, $\boldsymbol{\Delta} = \operatorname{diag}(\Delta, \ldots, \Delta)$ is the vector Laplacian with inverse $\boldsymbol{\Delta}^{-1} = \operatorname{diag}(\Delta^{-1}, \ldots, \Delta^{-1})$, $\langle \cdot \rangle$ denotes space-time averaging over the period cell $\mathcal{T} \times \mathcal{V}$, and I is the identity operator on $\mathcal{H}_{\mathcal{V}}$. Due to the *curl-free* vector field $\boldsymbol{\nabla}\chi_j$ at the heart of the cell problem in equation (2.8), we will find particular use of the Hilbert space $\mathcal{H}_\times$, which we define as

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

where we have denoted $\boldsymbol{\Gamma}_\times$ by $\boldsymbol{\Gamma}$ for notational simplicity. Since $(-\Delta)^{-1}$ is self-adjoint on $\mathcal{H}_\times$ [82], it is clear from integration by parts that $\boldsymbol{\Gamma}$ 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 $\mathcal{H}_\times$ [84, 76]. Analogous to equation (C.3), we define the Hilbert space $\mathcal{H}$ and its everywhere dense subset $\mathcal{F}$,

$$\mathcal{H}=\mathcal{H}_\mathcal{T}\otimes\mathcal{H}_\times,\qquad \mathcal{F}=\tilde{\mathcal{A}}_\mathcal{T}\otimes\mathcal{H}_\times. \tag{C.11}$$

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 $\langle\boldsymbol{\psi},\boldsymbol{\varphi}\rangle=\langle\boldsymbol{\psi}\cdot\boldsymbol{\varphi}\rangle$ with $\langle\boldsymbol{\psi},\boldsymbol{\varphi}\rangle=\overline{\langle\boldsymbol{\varphi},\boldsymbol{\psi}\rangle}$. We will henceforth assume that $\boldsymbol{u},\boldsymbol{\nabla}\chi_j\in\mathcal{F}$. In the case of a steady fluid velocity field $\boldsymbol{u}(\boldsymbol{x})$, we set $\mathcal{H}\equiv\mathcal{F}\equiv\mathcal{H}_\times$.

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

$$\boldsymbol{u}=\boldsymbol{\nabla}\cdot\mathsf{H},\qquad \mathsf{H}^T=-\mathsf{H}, \tag{C.12}$$

where H^T denotes transposition of the matrix H. Since $\boldsymbol{u}\in\mathcal{F}$, we have that the space-time periodic components H_{jk} of the matrix 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 $\mathcal{T}$ [12]. Due to the skew-symmetry of H, we have the identity $[\boldsymbol{\nabla}\cdot\mathsf{H}\,]\cdot\boldsymbol{\nabla}f=\boldsymbol{\nabla}\cdot[\mathsf{H}\boldsymbol{\nabla}f]$. Using this identity and the representation of the velocity field $\boldsymbol{u}$ in (C.12), the advection-diffusion equation in (2.1) can be written as a diffusion equation [28],

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

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

$$\mathsf{D}_{jk}=\varepsilon\delta_{jk}+\mathsf{H}_{jk},\quad j,k=1,\ldots,d. \tag{C.14}$$

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

$$\partial_\tau\chi_j=\boldsymbol{\nabla}_\xi\cdot[\mathsf{D}(\boldsymbol{\nabla}_\xi\chi_j+\boldsymbol{e}_j)],\quad \langle\boldsymbol{\nabla}_\xi\chi_k\rangle=0,\qquad \mathsf{D}=\varepsilon\mathsf{I}+\mathsf{H}, \tag{C.15}$$

where $\langle\boldsymbol{\nabla}_\xi\chi_k\rangle=0$ follows from the periodicity of χ_k. We stress that equation (C.13) involves the slow $(t,\boldsymbol{x})$ and fast variables $(\tau,\boldsymbol{\xi})$, while equation (C.15) involves only the fast variables. For notational simplicity, we will drop the subscripts ξ displayed in equation (C.15).

We now recast the first formula in equation (C.15) in a more suggestive, divergence form. Define the operator $\mathbf{T}:\tilde{\mathcal{A}}_\mathcal{T}\to\mathcal{H}_\mathcal{T}$ by $(\mathbf{T}\boldsymbol{\psi})_j=\partial_\tau\psi_j$, $j=1,\ldots,d$. For $f\in\mathscr{F}$ we have [28, 33]

$$\boldsymbol{\nabla}(\Delta^{-1})\partial_\tau f=\boldsymbol{\Delta}^{-1}\mathbf{T}\boldsymbol{\nabla}f, \tag{C.16}$$

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

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

The formulas in (C.17) are the quasi-static limit of Maxwell's equations for a conductive medium [35, 60], where $\boldsymbol{E}_k$ and $\boldsymbol{J}_k$ are the local electric field and current density, respectively, and $\boldsymbol{\sigma}$ is the local conductivity tensor of the medium. In the analytic continuation method for composites [35], the effective conductivity tensor $\boldsymbol{\sigma}^*$ is defined as

$$\langle\boldsymbol{J}_k\rangle=\boldsymbol{\sigma}^*\langle\boldsymbol{E}_k\rangle. \tag{C.18}$$

The linear constitutive relation $\boldsymbol{J}_k=\boldsymbol{\sigma}\boldsymbol{E}_k$ in (C.17) relates the local intensity and flux, while that in (C.18) relates the mean intensity and flux. Due to the skew-symmetry of $\mathbf{S}$, the intensity-flux relationship in (C.17) is similar to that of a Hall medium [42, 28]. We will explore the relationship between the effective parameters D^* and $\boldsymbol{\sigma}^*$ in more detail in Section C.3 below.

Analogous to equation (2.11), the components S^*_{jk} and A^*_{jk}, $j,k=1,\ldots,d$, of the symmetric S^* and antisymmetric A^* parts of the effective diffusivity tensor D^* can be represented by the following functional formulas in terms of the $\mathcal{H}$–inner-product $\langle\cdot,\cdot\rangle$,

$$\mathsf{S}^*_{jk}=\varepsilon(\delta_{jk}+\langle\boldsymbol{\nabla}\chi_j,\boldsymbol{\nabla}\chi_k\rangle),\qquad \mathsf{A}^*_{jk}=\langle\mathbf{A}\boldsymbol{\nabla}\chi_j,\boldsymbol{\nabla}\chi_k\rangle,\qquad \mathbf{A}=\boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}. \tag{C.19}$$

Equation (C.19) follows from the formula $\mathsf{D}^*_{jk}=\varepsilon\delta_{jk}+\langle u_j,\chi_k\rangle$ in equation (2.9) and the cell problem in equation (C.17) written as $\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_j=-\boldsymbol{\nabla}\cdot\mathsf{H}\boldsymbol{e}_j=-u_j$, yielding

$$\langle u_j,\chi_k\rangle=-\langle[\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_j],\chi_k\rangle=\langle\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_j,\boldsymbol{\nabla}\chi_k\rangle=\varepsilon\langle\boldsymbol{\nabla}\chi_j,\boldsymbol{\nabla}\chi_k\rangle+\langle\boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle, \tag{C.20}$$

where we have used the periodicity of χ_k and H in the second equality and the final equality follows from the property $\boldsymbol{\Gamma}\boldsymbol{\nabla}\chi_j=\boldsymbol{\nabla}\chi_j$. Since $\boldsymbol{\nabla}\chi_k$ is real-valued, we have that $\langle\boldsymbol{\nabla}\chi_k,\boldsymbol{\nabla}\chi_j\rangle=\langle\boldsymbol{\nabla}\chi_j,\boldsymbol{\nabla}\chi_k\rangle$, implying that S^* is indeed a symmetric matrix. As in Section C.1, we have $(-\boldsymbol{\Delta})^{-1}\mathbf{T}\boldsymbol{\psi}=\mathbf{T}(-\boldsymbol{\Delta})^{-1}\boldsymbol{\psi}$ for $\boldsymbol{\psi}\in\mathcal{F}$ [33, 82]. This and the skew-symmetry of the matrix H implies that $\mathbf{S}=\mathsf{H}+(-\boldsymbol{\Delta}^{-1})\mathbf{T}$ is a skew-symmetric operator on $\mathcal{F}$. Since, $\boldsymbol{\Gamma}$ is self-adjoint on $\mathcal{F}$, $\boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}$ is also skew-symmetric on $\mathcal{F}$. Just as in Section C.1, this implies that A^* is indeed an antisymmetric matrix. Analogous to equation (2.12) we have the following resolvent formula for $\boldsymbol{\nabla}\chi_j$

$$\boldsymbol{\nabla}\chi_j=(\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_j,\qquad \boldsymbol{g}_j=-\boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_j. \tag{C.21}$$

Equation (C.21) follows from applying the integro-differential operator $\boldsymbol{\nabla}(\Delta^{-1})$ to the cell problem in equation (C.17) written as $\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_j=-\boldsymbol{\nabla}\cdot\mathsf{H}\boldsymbol{e}_j$, yielding

$$\boldsymbol{\Gamma}(\varepsilon\mathsf{I}+\mathbf{S})\boldsymbol{\nabla}\chi_j=-\boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_j. \tag{C.22}$$

The equivalence of equations (C.21) and (C.22) then follows from the formula $\boldsymbol{\Gamma}\boldsymbol{\nabla}\chi_j=\boldsymbol{\nabla}\chi_j$. Inserting the resolvent formula for $\boldsymbol{\nabla}\chi_j$ in (C.21) into equation (C.19) yields the following analogue of (2.13)

$$\mathsf{S}^*_{jk}=\varepsilon\left(\delta_{jk}+\langle(\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_j,(\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_k\rangle\right),\quad \mathsf{A}^*_{jk}=\langle\mathbf{A}(\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_j,(\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_k\rangle, \tag{C.23}$$

We therefore have the following corollary of Theorem C.1.

Corollary C.3. *The operator $\mathbf{A}=\boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}$ with $\mathbf{S}=\mathbf{H}+(-\boldsymbol{\Delta})^{-1}\mathbf{T}$, displayed in equation* (C.19) *is a maximal (skew-symmetric) normal operator on the function space $\mathcal{F}$ defined in* (C.9)*, 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 $\mu_{jk}(\lambda)=\langle\mathbf{Q}(\lambda)\boldsymbol{g}_j,\boldsymbol{g}_k\rangle_1$, $j,k=1,\ldots,d$, where $\boldsymbol{g}_j=-\boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_j$ is defined in* (C.21) *and $\langle\cdot,\cdot\rangle$ is the $\mathcal{H}$–inner-product. Consider the positive measure μ_{kk} and the signed measures $Re\,\mu_{jk}$ and $Im\,\mu_{jk}$ associated with $\mu_{jk}(\lambda)$, introduced in equation* (A.5)*. Then, for $\boldsymbol{u},\boldsymbol{\nabla}\chi_j\in\mathcal{F}$ and all $0<\varepsilon<\infty$, the functional formulas for S^*_{jk} and A^*_{jk} displayed in* (C.23) *have the Radon–Stieltjes integral representations displayed in equation* (2.14).

Proof of Corollary C.3. We first establish that $\mathbf{M}=-\imath\mathbf{A}$, with $\mathbf{A}=\boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}$, is a self-adjoint operator on $\mathcal{F}$. Since $\boldsymbol{\Gamma}:\mathcal{H}_{\mathcal{V}}\to\mathcal{H}_\times$ is a projection, it acts as the identity on $\mathcal{H}_\times$. We can therefore focus our analysis on the operator $\mathbf{S}=\mathbf{H}+(-\boldsymbol{\Delta})^{-1}\mathbf{T}$. As discussed above, since $\boldsymbol{u}\in\mathcal{F}$ and $\boldsymbol{u}=\boldsymbol{\nabla}\cdot\mathbf{H}$, the skew-symmetric matrix $\mathbf{H}$ is bounded in operator norm $\|\mathbf{H}\|<\infty$ with domain $\tilde{\mathcal{A}}_{\mathcal{T}}\otimes\mathcal{H}_{\mathcal{V}}$, and is therefore a maximal (skew-symmetric) normal operator on the same domain [84]. It is clear from Section B that $-\imath\mathbf{T}$ is self-adjoint with domain $\tilde{\mathcal{A}}_{\mathcal{T}}$. The integral operator $(-\boldsymbol{\Delta})^{-1}$ is self-adjoint and compact on $\mathcal{H}_{\mathcal{V}}$. Since they commute on $\tilde{\mathcal{A}}_{\mathcal{T}}\otimes\mathcal{H}_{\mathcal{V}}$ [33], it follows that the operator $-\imath(-\boldsymbol{\Delta})^{-1}\mathbf{T}$ is self-adjoint with domain $\tilde{\mathcal{A}}_{\mathcal{T}}\otimes\mathcal{H}_{\mathcal{V}}$, hence $(-\boldsymbol{\Delta})^{-1}\mathbf{T}$ is a maximal (skew-symmetric) normal operator on the same domain.

Since $\boldsymbol{\Gamma}$ is bounded and self-adjoint on $\mathcal{H}_\times$, it follows that $\boldsymbol{\Gamma}\mathbf{H}\boldsymbol{\Gamma}$ is a maximal (skew-symmetric) normal operator on $\tilde{\mathcal{A}}_{\mathcal{T}}$. $\mathbf{A}=\boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}$, with $\mathbf{S}=\mathbf{H}+(-\boldsymbol{\Delta})^{-1}\mathbf{T}$ is a maximal (skew-symmetric) normal operator on $\mathcal{F}$. Consequently, $\mathbf{M}=-\imath\mathbf{A}$ is *self-adjoint* on $\mathcal{F}$.

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C.3. Effective diffusivity and the analytic continuation method. The following theorem provides the relationship of the effective parameters $\boldsymbol{\sigma}^*$ and D^* defined in equations (**??**) and (**??**), respectively

THEOREM C.4. *Let the components D^*_{jk} and σ^*_{jk}, $j,k=1,\ldots,d$, of the effective tensors D^* and $\boldsymbol{\sigma}^*$ be defined as in equations* (2.8)–(C.19) *and* (C.17)–(C.18), *respectively. Then for $\boldsymbol{\nabla}\chi_j\in\mathcal{F}$, D^*_{jk} and σ^*_{jk} are well defined and finite. Moreover, these effective tensors related by*

$$\boldsymbol{\sigma}^*=[\mathsf{D}^*]^T. \tag{C.24}$$

In particular, the symmetric part D^* of D^* is equal to that of $\boldsymbol{\sigma}^*$ and the anti-symmetric part A^* of D^* is equal to the negative of that of $\boldsymbol{\sigma}^*$. We defer the proof of Theorem C.4 to Section C.3.

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

$$\mathcal{F}=\{\boldsymbol{\psi}\in\mathcal{F}_\mathcal{T}\otimes\mathcal{H}_\times \mid \langle\boldsymbol{\psi}\rangle=0\}, \tag{C.25}$$

which will be used extensively. We stress that $\mathcal{F}$ is *not* a Hilbert space, and is instead a dense subset of the Hilbert space $\mathcal{H}_\mathcal{T}\otimes\mathcal{H}_\times$. We will henceforth assume that $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$. In the case of a time-independent velocity field $\boldsymbol{u}$ we set $\mathcal{F}_\mathcal{T}=\emptyset$ in (C.25), so that $\boldsymbol{\psi}\in\mathcal{F}$ implies $\boldsymbol{\psi}\in\mathcal{H}_\times$ with $\langle\boldsymbol{\psi}\rangle=0$. To summarize, since $\boldsymbol{\sigma}$ is bounded on $\mathcal{F}$ and $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$, we have that the divergence-free vector field $\boldsymbol{J}_k=\boldsymbol{\sigma}\boldsymbol{e}_k$ is also bounded $\|\boldsymbol{J}_k\|<\infty$, thus $\boldsymbol{J}_k\in\mathcal{H}_\mathcal{T}\otimes\mathcal{H}_\bullet$.

By the mutual orthogonality of the Hilbert spaces $\mathcal{H}_\times$ and $\mathcal{H}_\bullet$ in equation (C.10), $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$, $\boldsymbol{J}_k\in\mathcal{H}_\mathcal{T}\otimes\mathcal{H}_\bullet$, and Fubini's theorem [33] imply that $\langle\boldsymbol{J}_j\cdot\boldsymbol{\nabla}\chi_k\rangle=0$ for every $j,k=1,\ldots,d$. This is trivially satisfied in the case of a time-independent velocity field $\boldsymbol{u}$, since in this case $\boldsymbol{\sigma}=\mathsf{D}$ is bounded so that $\boldsymbol{J}_j\in\mathcal{H}_\bullet$ for $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$. In either case, as $\boldsymbol{e}_k=\boldsymbol{\nabla}\chi_k+\boldsymbol{e}_k$, we have $\langle\boldsymbol{J}_j\cdot\boldsymbol{e}_k\rangle=\langle\boldsymbol{J}_j\cdot\boldsymbol{e}_k\rangle$. Equations (C.17) and (C.18) then imply that the components $\sigma^*_{jk}=\boldsymbol{\sigma}^*\boldsymbol{e}_j\cdot\boldsymbol{e}_k=\langle\boldsymbol{\sigma}\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle$ of the effective tensor $\boldsymbol{\sigma}^*$ can be expressed as $\sigma^*_{jk}=\langle\boldsymbol{\sigma}\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle$, with $\boldsymbol{\sigma}=\varepsilon\mathsf{I}+\mathbf{S}$ and $\mathbf{S}=\mathsf{H}-(\boldsymbol{\Delta}^{-1})\mathbf{T}$. Consequently,

$$\sigma^*_{jk}=\varepsilon\langle\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle+\langle\mathbf{S}\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle. \tag{C.26}$$

The property $\langle\boldsymbol{\nabla}\chi_k\rangle=0$ in (**??**), and equation (C.19) together imply that

$$\varepsilon\langle\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle=\varepsilon[\langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle+\langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{e}_k\rangle+\langle\boldsymbol{e}_j\cdot\boldsymbol{\nabla}\chi_k\rangle+\langle\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle]=\varepsilon(\langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle+\delta_{jk})=\mathsf{S}^*_{jk}. \tag{C.27}$$

From the definition of $\mathbf{S}=\mathsf{H}-(\boldsymbol{\Delta}^{-1})\mathbf{T}$ in equation (C.19) we have that $\mathbf{S}\boldsymbol{e}_j=\mathsf{H}\boldsymbol{e}_j$. Consequently, $\langle\mathbf{S}\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle=\langle\mathsf{H}\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle=0$, since by equation (**??**) the matrix H is (component-wise) mean-zero. Also, by the definition $\boldsymbol{u}=\boldsymbol{\nabla}\cdot\mathsf{H}$ in (C.12) and the periodicity of H and χ_k, we also have $\langle\mathsf{H}\boldsymbol{e}_j\cdot\boldsymbol{\nabla}\chi_k\rangle=-\langle u_j\chi_k\rangle$ via integration by parts. Therefore, by the skew-symmetry of $\mathbf{S}$ on $\mathcal{F}$, the symmetries $\mathsf{S}^*_{kj}=\mathsf{S}^*_{jk}$ and $\mathsf{A}^*_{kj}=-\mathsf{A}^*_{jk}$, and equations (C.19), (**??**), and (C.20), we have

$$\begin{aligned}\langle\mathbf{S}\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle&=\langle\mathbf{S}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle+\langle\mathbf{S}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{e}_k\rangle+\langle\mathbf{S}\boldsymbol{e}_j\cdot\boldsymbol{\nabla}\chi_k\rangle+\langle\mathbf{S}\boldsymbol{e}_j\cdot\boldsymbol{e}_k\rangle\\&=\mathsf{A}^*_{jk}-\langle\boldsymbol{\nabla}\chi_j\cdot\mathsf{H}\boldsymbol{e}_k\rangle+\langle\mathsf{H}\boldsymbol{e}_j\cdot\boldsymbol{\nabla}\chi_k\rangle\\&=\mathsf{A}^*_{jk}+\langle\chi_ju_k\rangle-\langle u_j\chi_k\rangle\\&=\mathsf{A}^*_{jk}+[\mathsf{A}^*_{kj}+\mathsf{S}^*_{kj}-\varepsilon\delta_{kj}]-[\mathsf{A}^*_{jk}+\mathsf{S}^*_{jk}-\varepsilon\delta_{jk}]\\&=-\mathsf{A}^*_{jk}.\end{aligned} \tag{C.28}$$

In summary, from equations (C.26)–(C.28) and the symmetries $\mathsf{S}^*_{jk}=\mathsf{S}^*_{kj}$ and $\mathsf{A}^*_{jk}=-\mathsf{A}^*_{kj}$ we have that

$$\sigma^*_{jk}=\mathsf{S}^*_{jk}-\mathsf{A}^*_{jk}=\mathsf{S}^*_{kj}+\mathsf{A}^*_{kj}=\mathsf{D}^*_{kj}\,, \tag{C.29}$$

which is equivalent to equation (C.24). This concludes our proof of Theorem C.4 □.

Appendix D. Need this to prove.

Proof of Corollary C.3. We first note that from $\boldsymbol{\nabla}\chi_k \in \mathcal{F}$ we have $\boldsymbol{\nabla}\chi_k = \boldsymbol{\Gamma}\boldsymbol{\nabla}\chi_k$, so that A^*_{jk} in equation (C.19) can re-expressed as $\mathsf{A}^*_{jk} = \langle \mathbf{S}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle \boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle \mathbf{A}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle$, where we have used that $\boldsymbol{\Gamma}$ is self-adjoint on $\mathcal{F}$. From this and (C.21), equation (C.19) can be rewritten as

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

where $\boldsymbol{g}_k = -\boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_k$. The integral representations for S^*_{jk} and A^*_{jk} in (2.14) follow from equations (A.7) and (C.23), and the symmetries $\langle\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle\boldsymbol{\nabla}\chi_k \cdot \boldsymbol{\nabla}\chi_j\rangle$ and $\langle\mathbf{A}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle\boldsymbol{\nabla}\chi_k \cdot \mathbf{A}\boldsymbol{\nabla}\chi_j\rangle$, since $\boldsymbol{\nabla}\chi_k$ and $\mathbf{A}\boldsymbol{\nabla}\chi_k$ are real-valued. We prove the validity of (2.14) by showing that the conditions of the spectral theorem of equation (A.7) are satisfied for the functionals in (C.23) and then employing these symmetries.

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

Consider the representation for S^*_{jk} in (C.23) and define the function $F(z) = (\varepsilon+z)^{-1}$ so that, formally, $\mathsf{S}^*_{jk} = \varepsilon(\delta_{jk} + \langle F(\mathbf{A})\boldsymbol{g}_j \cdot F(\mathbf{A})\boldsymbol{g}_k\rangle)$. Since $\boldsymbol{g}_k \in \mathcal{F}$ for all $k = 1,\dots,d$, once we establish that $\boldsymbol{g}_k \in \mathscr{D}(F)$, i.e. $F \in L^2(\mu_{kk})$, the integral representations for S^*_{jk}, $j,k = 1,\dots,d$, in (2.14) follow from the second formula in (A.7) with $F(z) = G(z) = (\varepsilon+z)^{-1}$, $\boldsymbol{\psi} = \boldsymbol{g}_j$, and $\boldsymbol{\varphi} = \boldsymbol{g}_k$. Since $0 < \varepsilon < \infty$ and $z \in (-\imath\infty, \imath\infty)$ for the anti-symmetric operator $\mathbf{A}$, the function $|F(z)|^2 = |\varepsilon+z|^{-2}$ is bounded, and the validity of $F \in L^2(\mu_{kk})$ is an immediate consequence of the boundedness of the (positive) measure mass $\mu^0_{kk} = \int \mathrm{d}\mu_{kk}(z) < \infty$. The validity of $\mu^0_{kk} < \infty$, in turn, is a consequence of the fact that the function $\mu_{jk}(z) = \langle\mathbf{Q}(z)\boldsymbol{g}_j \cdot \boldsymbol{g}_k\rangle$ is of *bounded variation* when $\boldsymbol{g}_j, \boldsymbol{g}_k \in \mathcal{F}$, hence $|\mu^0_{jk}| < \infty$ for all $j,k = 1,\dots,d$ [84]. We have therefore established that $\boldsymbol{g}_k \in \mathscr{D}(F)$ for all $k = 1,\dots,d$.

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

$$\mu^0_{jk} = \int_{-\infty}^{\infty} \mathrm{d}\langle\mathbf{Q}(z)\boldsymbol{g}_j, \boldsymbol{g}_k\rangle = \langle\boldsymbol{g}_j, \boldsymbol{g}_k\rangle = \langle\boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_j \cdot \boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_k\rangle = \langle\mathsf{H}^T\boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_j \cdot \boldsymbol{e}_k\rangle. \tag{D.2}$$

This and equation (**??**) imply that $|\mu^0_{jk}| \le \|\mathsf{H}\|^2 < \infty$ for all $j,k = 1,\dots,d$.

This concludes our proof of Theorem C.1 □.

D.1. An isometric correspondence. A natural question to ask is the following. Is the formulation of the effective parameter problem described in Theorem C.4 equivalent to that described in Corollary C.3? The correspondence between the two formulations is one of isometry, and is summarized by the following theorem.

Theorem D.1. *The function spaces $\mathcal{F}$ and $\mathscr{F}$ defined in equations* (C.25) *and* (C.3) *are in one-to-one isometric correspondence. This induces a one-to-one isometric correspondence between the domains $D(\mathbf{A})$ and $D(A)$ of the operators $\mathbf{A}$ and A defined in equations* (C.21) *and* (2.11)*, respectively. Specifically, for every $f \in D(A)$ we have $\boldsymbol{\nabla}f \in D(\mathbf{A})$ and $\|Af\|_1 = \|\mathbf{A}\boldsymbol{\nabla}f\|$, and conversely, for each $\boldsymbol{\psi} \in D(\mathbf{A})$ there exists unique $f \in D(A)$ such that $\boldsymbol{\psi} = \boldsymbol{\nabla}f$ and $\|\mathbf{A}\boldsymbol{\psi}\| = \|Af\|_1$. The Radon–Stieltjes measures underlying the integral representations of Theorem C.4 and Corollary C.3 are equal, $\mathrm{d}\langle Q_2(\lambda)g_j, g_k\rangle_1 = \mathrm{d}\langle\mathbf{Q}_2(\lambda)\boldsymbol{g}_j, \boldsymbol{g}_k\rangle$, $j,k = 1,\dots,d$, up to null sets of measure zero, where $\boldsymbol{g}_j = \boldsymbol{\nabla}g_j$. Moreover, the operators $\mathbf{A}$ and A are related by $\mathbf{A}\boldsymbol{\nabla} = \boldsymbol{\nabla}A$, which implies and is implied by the weak equality $\mathbf{Q}_2(\lambda)\boldsymbol{\nabla} = \boldsymbol{\nabla}Q_2(\lambda)$.*

Proof of Theorem D.1. We use the formula $\boldsymbol{u} = \boldsymbol{\nabla}\cdot\mathsf{H}$ displayed in equation (C.12) to write the operator $A = \Delta^{-1}(\boldsymbol{u}\cdot\boldsymbol{\nabla} - \partial_t)$ and function $g_j = (-\Delta)^{-1}u_j$ defined in equations (2.11) and (2.12) as $A = \Delta^{-1}(\boldsymbol{\nabla}\cdot\mathsf{H}\boldsymbol{\nabla} - \partial_t)$ and $g_j = (-\Delta)^{-1}\boldsymbol{\nabla}\cdot\mathsf{H}\boldsymbol{e}_j$, respectively. Using the definition $\boldsymbol{\Gamma} = \boldsymbol{\nabla}(\Delta^{-1})\boldsymbol{\nabla}\cdot$ and the formulas $\boldsymbol{\nabla}\Delta^{-1}\partial_t = \boldsymbol{\Delta}^{-1}\mathbf{T}\boldsymbol{\nabla}$, $\boldsymbol{g}_j = -\boldsymbol{\Gamma}\mathsf{H}\boldsymbol{e}_j$, and $\mathbf{A} = \boldsymbol{\Gamma}\mathsf{H} - \boldsymbol{\Delta}^{-1}\mathbf{T}$ displayed in equations, (C.21), and (C.22), respectively, we have that

$$\boldsymbol{\nabla}A = [\boldsymbol{\Gamma}\mathsf{H} - \boldsymbol{\Delta}^{-1}\mathbf{T}]\boldsymbol{\nabla} = \mathbf{A}\boldsymbol{\nabla}, \qquad \boldsymbol{\nabla}g_j = \boldsymbol{g}_j. \tag{D.3}$$

Consequently, by applying the differential operator $\boldsymbol{\nabla}$ to both sides of the formula $(\varepsilon + A)\chi_j = g_j$ of (2.12), we obtain the formula $(\varepsilon \mathsf{I} + \mathbf{A})\boldsymbol{\nabla}\chi_j = \boldsymbol{g}_j$ of equation (C.21).

Since the function spaces $\mathscr{F}$ and $\mathcal{F}$ differ only in the characterization of the spatial variable $\boldsymbol{x}$, we now discuss the relationship between the Hilbert spaces $\mathcal{H}_\times$ and $\mathscr{H}^1_\mathcal{V}$ defined in equations (C.10) and (C.2), respectively, with inner-product induced norms $\|\cdot\|$ and $\|\cdot\|_1$. For $f \in \mathscr{H}^1_\mathcal{V} \subset L^2(\mathcal{V})$ we have $\Delta^{-1}\Delta f = f$ [82], which implies that $\boldsymbol{\Gamma}\boldsymbol{\nabla} f = \boldsymbol{\nabla} f$ and $\|\boldsymbol{\nabla} f\|^2 = \langle \boldsymbol{\nabla} f \cdot \boldsymbol{\nabla} f\rangle = \|f\|_1^2 < \infty$. Consequently, for every $f \in \mathscr{H}^1_\mathcal{V}$ we have $\boldsymbol{\nabla} f \in \mathcal{H}_\times$. Conversely, $\boldsymbol{\psi} \in \mathcal{H}_\times$ implies that $\boldsymbol{\psi} = \boldsymbol{\Gamma}\boldsymbol{\psi} = \boldsymbol{\nabla} f$, where we have defined the scalar-valued function $f = \Delta^{-1}\boldsymbol{\nabla}\cdot\boldsymbol{\psi}$. Since $\boldsymbol{\psi} = \boldsymbol{\nabla} f$, the $\mathscr{H}^1_\mathcal{V}$ norm of f satisfies $\|f\|_1^2 = \langle \boldsymbol{\psi}\cdot\boldsymbol{\psi}\rangle = \|\boldsymbol{\psi}\|^2 < \infty$ so that $f \in \mathscr{H}^1_\mathcal{V}$. Moreover, f is uniquely determined by $\boldsymbol{\psi}$ up to equivalence class, since if $f_1 = \Delta^{-1}\boldsymbol{\nabla}\cdot\boldsymbol{\psi}$ and $f_2 = \Delta^{-1}\boldsymbol{\nabla}\cdot\boldsymbol{\psi}$ then $\boldsymbol{\Gamma}\boldsymbol{\psi} = \boldsymbol{\psi}$ implies that $\|f_1 - f_2\|_1 = \|\boldsymbol{\psi} - \boldsymbol{\psi}\| = 0$. Consequently, for every $\boldsymbol{\psi} \in \mathcal{H}_\times$ there exists unique $f \in \mathscr{H}^1_\mathcal{V}$ such that $\boldsymbol{\psi} = \boldsymbol{\nabla} f$. In summary, the Hilbert spaces $\mathscr{H}^1_\mathcal{V}$ and $\mathcal{H}_\times$ are in one-to-one isometric correspondence, which we denote by $\mathscr{H}^1_\mathcal{V} \sim \mathcal{H}_\times$. This, in turn, implies $\mathscr{F} \sim \mathcal{F}$.

We now return to our previous notation, where $\|\cdot\|_1$ and $\|\cdot\|$ denotes the norm induced by the $\mathscr{F}$- and $\mathcal{F}$–inner-product, respectively. We demonstrate that the one-to-one isometry between $\mathscr{F}$ and $\mathcal{F}$ induces a one-to-one isometry between the domains $D(A)$ and $D(\mathbf{A})$ of the operators A and $\mathbf{A}$, i.e. $D(A) \sim D(\mathbf{A})$. This, in turn, follows from another on-to-one isometry between the class of self-adjoint operators on $\mathscr{F}$, for example, and the class of resolutions of the identity. This correspondence is determined directly as follows [84]. Let X be a self-adjoint operator on $\mathscr{F}$ and $Q(\lambda)$ be the associated resolution of the identity, which is a one-to-one correspondence [84]. The domain $D(X)$ of X comprises those and only those elements $f \in \mathscr{F}$ such that the Stieltjes integral $\int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}\|Q(\lambda)f\|_1^2$ is convergent; when $f \in D(X)$ the element Xf is determined by the relations

$$\langle Xf, h\rangle_1 = \int_{-\infty}^{\infty}\lambda\,\mathrm{d}\langle Q(\lambda)f, h\rangle_1, \qquad \|Xf\|_1^2 = \int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}\|Q(\lambda)f\|_1^2, \tag{D.4}$$

where h is an arbitrary element in $\mathscr{F}$ [84]. Since $M = -\imath A$ is self-adjoint on $\mathscr{F}$ and $D(A) = D(M)$, this one-to-one isometric correspondence also holds for the maximal normal operator A, and a calculation similar to that in equations (**??**) and (**??**) shows that equation (A.11) holds under the mappings $X \mapsto A$, $\lambda\,\mathrm{d}\langle Q(\lambda)f, h\rangle_1 \mapsto \lambda\,\mathrm{d}\mathrm{Im}\,\langle Q(\lambda)f, h\rangle_1$, and $Q(\lambda) \mapsto Q_2(\lambda)$. An analogous result holds for the self-adjoint operator $\mathbf{M} = -\imath\mathbf{A}$ on $\mathcal{F}$ with $D(\mathbf{A}) = D(\mathbf{M})$.

We now demonstrate that the one-to-one isometry between the class of self-adjoint operators and resolutions of the identity on $\mathscr{F}$, and that for $\mathcal{F}$, along with the property $\mathscr{F} \sim \mathcal{F}$ and equation (D.3), induce the one-to-one isometry $D(A) \sim D(\mathbf{A})$. From $\mathscr{F} \sim \mathcal{F}$, we have for every $f \in D(A) \subset \mathscr{F}$ that $\boldsymbol{\nabla} f \in \mathcal{F}$, so from equation (D.3)

$$\|Af\|_1^2 = \langle Af, Af\rangle_1 = \langle \boldsymbol{\nabla} Af \cdot \boldsymbol{\nabla} Af\rangle = \langle \mathbf{A}\boldsymbol{\nabla} f \cdot \mathbf{A}\boldsymbol{\nabla} f\rangle = \|\mathbf{A}\boldsymbol{\nabla} f\|^2. \tag{D.5}$$

Consequently, from equation (A.11) we have

$$\int \lambda^2\,\mathrm{d}\|Q_2(\lambda)f\|_1^2 = \int \lambda^2\,\mathrm{d}\|\mathbf{Q}_2(\lambda)\boldsymbol{\nabla} f\|^2, \tag{D.6}$$

and the convergence of the left-hand-side of (D.6) implies the convergence of the right-hand-side which, in turn, implies that $\boldsymbol{\nabla} f \in D(\mathbf{A})$. Conversely, from $\mathscr{F} \sim \mathcal{F}$ we have that $\boldsymbol{\psi} \in D(\mathbf{A}) \subset \mathcal{F}$ implies there exists unique $f \in \mathscr{F}$ such that $\boldsymbol{\psi} = \boldsymbol{\nabla} f$, and equation (D.3) then implies that

$$\|\mathbf{A}\boldsymbol{\psi}\|^2 = \langle \mathbf{A}\boldsymbol{\nabla} f, \mathbf{A}\boldsymbol{\nabla} f\rangle = \langle \boldsymbol{\nabla} Af, \boldsymbol{\nabla} Af\rangle = \langle Af, Af\rangle_1 = \|Af\|_1^2. \tag{D.7}$$

Again, equation (A.11) implies that (D.6) holds, and the convergence of the right-hand-side of (D.6) implies the convergence of the left-hand-side which, in turn, implies that $f \in D(A)$. In summary, for every $f \in D(A)$ we have $\boldsymbol{\nabla} f \in D(\mathbf{A})$ and $\|Af\|_1^2 = \|\mathbf{A}\boldsymbol{\nabla} f\|^2$. Conversely, for each $\boldsymbol{\psi} \in D(\mathbf{A})$ there exists unique $f \in D(A)$ such that $\boldsymbol{\psi} = \boldsymbol{\nabla} f$ and $\|\mathbf{A}\boldsymbol{\psi}\|^2 = \|Af\|_1^2$. Consequently, the domains $D(\mathbf{A})$ and $D(A)$ are in one-to-one isometric correspondence, i.e. $D(\mathbf{A}) \sim D(A)$.

We now show that this result implies, and is implied by the weak equality $\boldsymbol{\nabla} Q_2(\lambda) = \mathbf{Q}_2(\lambda)\boldsymbol{\nabla}$, where $Q_2(\lambda)$ and $\mathbf{Q}_2(\lambda)$ are the resolutions of the identity associated with the operators A and $\mathbf{A}$, respectively. From equation (D.6) and the linearity properties of Radon–Stieltjes integrals [84], we have that

$$0 = \int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}(\|Q_2(\lambda)f\|_1^2 - \|\mathbf{Q}_2(\lambda)\boldsymbol{\nabla} f\|^2) = \int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}(\langle[\boldsymbol{\nabla} Q_2(\lambda) - \mathbf{Q}_2(\lambda)\boldsymbol{\nabla}]f\cdot\boldsymbol{\nabla} f\rangle). \tag{D.8}$$

Equation (D.8) implies that for all $f \in D(A) \iff \boldsymbol{\nabla} f \in D(\mathbf{A})$ we have $\mathrm{d}\|Q_2(\lambda)f\|_1^2 = \mathrm{d}\|\mathbf{Q}_2(\lambda)\boldsymbol{\nabla} f\|^2$, up to null sets of measure zero. Moreover, the equality $\boldsymbol{\nabla} Q_2(\lambda) = \mathbf{Q}_2(\lambda)\boldsymbol{\nabla}$ holds weakly. Conversely, assume that $Q_2(\lambda)$ and $\mathbf{Q}_2(\lambda)$ are the resolutions of the identity associated with the operators A and $\mathbf{A}$ on the function spaces $\mathscr{F}$ and $\mathcal{F}$, respectively, which is a one-to-one correspondence [84], and that $\boldsymbol{\nabla} Q_2(\lambda)f = \mathbf{Q}_2(\lambda)\boldsymbol{\nabla} f$ holds for every $f \in D(A) \iff \boldsymbol{\nabla} f \in D(\mathbf{A})$. Then equation (D.8) holds and implies equation (D.6). The correspondence $D(A) \sim D(\mathbf{A})$ and equation (A.11) then imply that $\|\mathbf{A}\boldsymbol{\nabla} f\|^2 = \|Af\|_1^2 = \|\boldsymbol{\nabla} Af\|^2$, hence $\|(\mathbf{A}\boldsymbol{\nabla} - \boldsymbol{\nabla} A)f\|^2 = 0$ for every $f \in D(A) \iff \boldsymbol{\nabla} f \in D(\mathbf{A})$, which implies that $\mathbf{A}\boldsymbol{\nabla} = \boldsymbol{\nabla} A$ weakly. Since $g_k \in D(A)$ and $\boldsymbol{g}_k \in D(\mathbf{A})$ with $\boldsymbol{g}_k = \boldsymbol{\nabla} g_k$, this result implies that the Radon–Stieltjes measures underlying the integral representations of Theorem C.4 and Corollary C.3 are equal $\mathrm{d}\langle Q_2(\lambda)g_j, g_k\rangle_1 = \mathrm{d}\langle \mathbf{Q}_2(\lambda)\boldsymbol{g}_j, \boldsymbol{g}_k\rangle$ up to null sets of measure zero, for all $j, k = 1, \ldots, d$. This concludes our proof of Theorem D.1 $\Box$.

D.2. Section Break Here. In Section C we provide two natural Hilbert space formulations of the effective parameter problem for advection enhanced diffusion, yielding integral representations for both the symmetric and antisymmetric parts of the effective diffusivity tensor D^*. This approach is based on the spectral theorem discussed in this section and resolvent formulas for the functions $\boldsymbol{\nabla}\chi_j$ and χ_j, introduced in equations (2.9) and (2.8), involving self-adjoint operators on appropriate Hilbert spaces. In Section D.1 we prove that the two formulations are equivalent, and follow from an one-to-one isometric correspondence between the underlying Hilbert spaces and the one-to-one correspondence between the operator and its resolution of the identity determined by equation (A.11). FINISH THIS PARAGRAPH AFTER SECTION Section C IS WRITTEN.

D.3. Discrete integral representations by eigenfunction expansion. The integral representations of Theorem C.1 and Corollary C.3 displayed in equation (2.14), involve a spectral measure μ_{jk}, $j, k = 1, \ldots, d$, which has discrete and continuous components [76, 84]. 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 $\mathscr{F}$ and $\mathcal{F}$, which are densely defined on the associated Hilbert spaces $\mathscr{H}$ and $\mathcal{H}$, given in equations (C.3) and (C.11), respectively. We will focus on the operator M and the Hilbert space $\mathscr{H}$, as the discussion regarding $\mathbf{M}$ and $\mathcal{H}$ is analogous.

Recall from equation (A.11) that the domain $D(M)$ of the self-adjoint operator M comprises those and only those elements $f \in \mathscr{H}$ such that $\|Mf\|_1^2 = \int_{-\infty}^{\infty} \lambda^2\, \mathrm{d}\|Q(\lambda)f\|_1^2 < \infty$, where $Q(\lambda)$ is the resolution of the identity in one-to-one correspondence with M [84]. The integration is over the spectrum Σ of M, which has continuous Σ_{cont} and discrete (pure-point) Σ_{pp} components, $\Sigma = \Sigma_{\mathrm{cont}} \cup \Sigma_{\mathrm{pp}}$ [76, 84]. We first focus on the discrete spectrum Σ_{pp}.

The $f \in \mathscr{H}$, $f \neq 0$, satisfying $Mf = \lambda f$ with $\lambda \in \Sigma_{\mathrm{pp}}$ are called eigenfunctions and λ is the corresponding eigenvalue. Since M is self-adjoint, λ is real-valued [84]. The span of all eigenfunctions is a *countable* subspace of $\mathscr{H}$ [84]. Accordingly, we will denote the eigenfunctions by φ_l, $l = 1, 2, 3, \ldots$, with corresponding eigenvalues λ_l. Eigenfunctions corresponding to distinct eigenvalues are orthogonal and can be normalized to be orthonormal [84], 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 [84]. 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 $\mathcal{E} = \oplus_{l=1}^{\infty}\mathcal{M}(\varphi_l)$, $\mathcal{M} = \mathcal{E} \oplus \{0\}$, and let $\mathcal{N} = \mathcal{M}^{\perp}$ be the orthogonal complement of $\mathcal{M}$ in $\mathscr{H}$. All the properties of $\mathcal{M}$ and $\mathcal{N}$ that are relevant here have been collected in the following theorem [84], which provides a natural decomposition of the Hilbert space $\mathscr{H}$ 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 D.2 ([84] pages 189 and 247). *One of the three cases must occur:*

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

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

3. *$\mathcal{E}$ contains a complete orthonormal set $\{\varphi_l\}$; $\mathcal{M} = \mathscr{H}$ 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 $\mathcal{M} = \oplus_{l=1}^{\infty}\mathcal{M}(\varphi_l)$.*

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 $\varphi_l \in \mathscr{H}$ 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 $\lambda_l < \lambda < \infty$ [84]. Moreover, a necessary and sufficient condition that $f \in \mathcal{M}$, $f \neq 0$, is

$$f = \sum_{l=1}^{\infty}\langle f, \varphi_l\rangle_1\, \varphi_l, \qquad \|f\|_1^2 = \sum_{l=1}^{\infty}|\langle f, \varphi_l\rangle_1|^2 \neq 0, \tag{D.9}$$

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 [84].

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

$$\|Q(\lambda)f\|_1^2 = \|Q(\lambda)g\|_1^2 + \|Q(\lambda)h\|_1^2, \qquad \mathrm{d}\|Q(\lambda)f\|_1^2 = \mathrm{d}\|Q(\lambda)g\|_1^2 + \mathrm{d}\|Q(\lambda)h\|_1^2 \tag{D.10}$$

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 $\mathrm{d}\|Q(\lambda)f\|_1^2$ into its discrete and continuous components.

We now use the mathematical framework summarized in Theorem D.2 to provide explicit formulas for the discrete parts of the integral representations for S_{jk}^* and A_{jk}^*, displayed in equation (2.14). Recall the cell problem in equation (2.8) written as in (C.4), $(\varepsilon + A)\chi_j = g_j$. Here $A = \imath M$ is defined in (2.11), $g_j = (-\Delta)^{-1}u_j$, and u_j is the j^{th} component of the velocity field $\boldsymbol{u}$, $j = 1, \dots, d$. Moreover, we have $\chi_j, g_j \in \mathscr{F} \subset \mathscr{H}$ and $\mathscr{F} \subset D(A)$. 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 [33]. However, for the operator A, we must instead rely on general principles of unbounded linear operators in Hilbert space.

Let $\tilde{\chi}_j$ and $\chi_j^{\perp}$ 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 D.2, 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 (D.9) we then have $A\tilde{\chi}_j = \sum_l \langle A\tilde{\chi}_j, \varphi_l\rangle_1\, \varphi_l$ and

$$\chi_j = \sum_l \langle \tilde{\chi}_j, \varphi_l\rangle_1\, \varphi_l + \chi_j^{\perp}, \quad A\chi_j = \sum_l \imath\lambda_l \langle \tilde{\chi}_j, \varphi_l\rangle_1\, \varphi_l + A\chi_j^{\perp} \tag{D.11}$$

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

$$\varepsilon\sum_l \langle \tilde{\chi}_j, \varphi_l\rangle_1\varphi_l + \sum_l \imath\lambda_l\langle \tilde{\chi}_j, \varphi_l\rangle_1\varphi_l + (\varepsilon + A)\chi_j^{\perp} = \tilde{g}_j + g_j^{\perp}, \tag{D.12}$$

where $(\varepsilon + A)\chi_j^{\perp}, g_j^{\perp} \in \mathcal{N}$. Of course, each $f \in \mathcal{N}$ can be represented [84] as $f = \sum_m \langle f, \psi_m\rangle_1\, \psi_m$, where $\{\psi_m\}$ is the orthonormal set defined in Theorem D.2, 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 (D.12) with φ_n yields

$$\langle \tilde{\chi}_j, \varphi_n\rangle_1 = \frac{\langle \tilde{g}_j, \varphi_n\rangle_1}{(\varepsilon + \imath\lambda_n)}, \quad 0 < \varepsilon < \infty. \tag{D.13}$$

Recall the representations $\mathsf{S}^*_{jk} = \varepsilon(\delta_{jk} + \langle \chi_j, \chi_k \rangle_1)$ and $\mathsf{A}^*_{jk} = \langle A\chi_j, \chi_k \rangle_1$, $j, k = 1, \ldots, d$, displayed in equation (2.11). 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 (D.11) and (D.13), the completeness of the set $\{\varphi_l\} \cup \{\psi_m\}$, and the Parseval identity, we have

$$\text{(D.14)} \qquad \langle \chi_j, \chi_k \rangle_1 - \langle \chi_j^\perp, \chi_k^\perp \rangle_1 = \sum_l \langle \tilde{\chi}_j, \varphi_l \rangle_1 \overline{\langle \tilde{\chi}_k, \varphi_l \rangle}_1 = \sum_l \frac{\langle \tilde{g}_j, \varphi_l \rangle_1 \overline{\langle \tilde{g}_k, \varphi_l \rangle}_1}{\varepsilon^2 + \lambda_l^2}$$

$$\langle A\chi_j, \chi_k \rangle_1 - \langle A\chi_j^\perp, \chi_k^\perp \rangle_1 = \sum_l \imath\lambda_l \, \langle \tilde{\chi}_j, \varphi_l \rangle_1 \overline{\langle \tilde{\chi}_k, \varphi_l \rangle}_1 = \sum_l \frac{\imath\lambda_l \, \langle \tilde{g}_j, \varphi_l \rangle_1 \overline{\langle \tilde{g}_k, \varphi_l \rangle}_1}{\varepsilon^2 + \lambda_l^2}\,.$$

The right hand sides of the formulas in equation (D.14) 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 $\mathrm{d}\langle Q(\lambda) g_j^\perp, g_k^\perp \rangle_1$ via equation (2.14). 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 $\langle g_j, \varphi_l \rangle_1 = \langle u_j, \varphi_l \rangle_2$ (see equation (C.5)). 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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