SPECTRAL ANALYSIS AND COMPUTATION OF EFFECTIVE DIFFUSIVITIES FOR TIME-DEPENDENT PERIODIC FLOWS

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

Key words. advective diffusion, effective diffusivity, eddy diffusivity, spectral measure, multiscale homogenization, turbulence, residual diffusion

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1. Introduction.

The long time, large scale motion of diffusing particles or tracers being advected by an incompressible flow field is equivalent to an enhanced diffusive process [87] 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 [47, 75, 18, 19, 17], turbulent combustion [3, 14, 86], and solute transport in porous media [11, 12, 91, 39, 48, 51, 49]. 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 [23, 38], turbulence plays a key role in transporting mass, heat, momentum, energy, and salt in geophysical flows [64]. Turbulence enhances the dispersion of atmospheric gases [25] such as ozone [41, 72, 73, 74] and pollutants [22, 9, 79], as well as atmosphere-ocean transfers of carbon dioxide and other climatically important trace gas fluxes [93, 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 [92, 50, 15]. Chaotic motion of time-dependent fluid velocity fields cause instabilities in large scale ocean currents, generating geostrophic eddies [29] which dominate the kinetic energy of the ocean [30]. Geostrophic eddies greatly enhance [29] 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 [82]. 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 [20]. In sea ice, which couples the atmosphere to the polar oceans [89], the transport of vast ice floes can also be enhanced by eddie fluxes [90, 53].

It has been noted in various geophysical contexts [73, 74] that eddy-induced, skew-diffusive tracer fluxes, directed normal to the tracer gradient [62], are generally equivalent to antisymmetric components in the effective diffusivity tensor D^*, while the symmetric part of D^* represents irreversible diffusive effects [76, 80, 37] directed down the tracer gradient. The mixing of eddy fluxes is typically non-divergent and unable to affect the evolution of the mean flow [62], and do not alter the tracer moments [37]. In this sense, the mixing is non-dissipative, reversible, and sometimes referred to as stirring [24, 37].

Due to the computational intensity of detailed climate models [38, 89, 67], 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 [52], atmospheric boundary layer turbulence [16], atmosphere-surface exchange over the sea [26] and sea ice [81, 1, 2, 88], and eddies in the ocean [58, 35]. In this way, only the effective or averaged behavior of these sub-grid processes are included in the models. Here, we study the effective behavior of advection enhanced diffusion by time-dependent fluid velocity fields, with possibly chaotic dynamics, which gives rise to such a parameterization, namely, the effective diffusivity tensor D^* of the flow.

In recent decades, a broad range of mathematical techniques have been developed which reduce the analysis of enhanced diffusive transport by complex fluid velocity fields with rapidly varying structures in both space and time, to solving averaged or *homogenized* equations that do not have rapidly varying data, and involve an effective parameter [68, 59, 8, 13, 27, 28, 57, 70, 71, 21, 40, 43, 55, 56]. Motivated by [69], it was shown [59] 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 [59]. 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 [59].

The incompressibility condition of the time-independent fluid velocity field was used [4, 5] to transform the cell problem in [59] into the quasi-static limit of Maxwell's equations [45, 36], which describe the transport properties of an electromagnetic wave in a composite material [63]. The analytic continuation method for representing transport in composites [36] provides Stieltjes integral representations for the bulk transport coefficients of composite media, such as electrical conductivity and permittivity, magnetic permeability, and thermal conductivity [63]. This method is based on the spectral theorem [85, 77] and a resolvent formula for, say, the electric field, involving a random self-adjoint operator [36, 66] or matrix [65]. Based on [36], the cell problem was transformed into a resolvent formula involving a *bounded* self-adjoint operator, acting on the Hilbert space of curl-free random vector fields [4, 5]. This, in turn, led to a Stieltjes integral representation for the symmetric part of the effective diffusivity tensor D^*, involving the Péclet number Pe of the flow and a *spectral measure* $\boldsymbol{\mu}$ 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, 27, 28].

The mathematical framework developed in [59] was adapted [70, 60] to the case of a periodic, time-dependent, incompressible fluid velocity field with *non-zero* mean. The velocity field was modeled as a superposition of a large-scale mean flow with small-scale periodically oscillating fluctuations. It was shown [70] that, depending on the strength of the fluctuations relative to the mean flow, the effective diffusivity tensor D^* can be constant or a function of both space and time. When D^* is constant, only its symmetric part appears in the homogenized equation as an enhancement in the diffusivity. However, when D^* is a function of space and time, its antisymmetric part also plays a key role in the homogenized equation. In particular, the symmetric part of D^* appears as an enhancement in the diffusivity, while both the symmetric and antisymmetric parts of D^* contribute to an effective drift in the homogenized equation. The effective drift due to the antisymmetric part is purely sinusoidal, thus divergence-free [70]. This is consistent with what has been observed in geophysical flows in the climate system, as discussed above. In [60], this result was extended to weakly compressible, anelastic fluid velocity fields.

Based on [11], the cell problem discussed in [70] was transformed into a resolvent formula involving a self-adjoint operator, acting on the Sobolev space [61, 31] 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 [11], hence *bounded* [83]. 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 adapt and extend both of the approaches described in [4, 5] and [70] to the case of a periodic, *time-dependent* fluid velocity field, allowing for chaotic dynamics. In particular, for each approach, we provide Stieltjes integral representations for both the symmetric and antisymmetric parts of the effective diffusivity tensor D^*, involving a spectral measure of a self-adjoint operator. In this time-dependent setting, the underlying operator becomes *unbounded*. The spectral theory of unbounded operators is more subtle and technically challanging than that of bounded operators. For example, the domain of an unbounded operator and its adjoint plays a central role in the spectral characterization of the operator. Neglecting such important mathematical details, the Stieltjes integral representation for D^* given in [4, 5] was extended to the time-dependent setting in [6]. Here, we provide a mathematically rigorous formulation of Stieltjes integral representations for D^* in the time-dependent, unbounded operator setting. We prove that the two approaches described in [4, 5] and [70] are equivalent in this setting, and that their correspondence follows from a one-to-one isometry between the underlying Hilbert spaces. We also establish a direct correspondence between the effective parameter problem for D^* and that arising in the analytic continuation method for composite media. Analytical calculations of the spectral measure underlying the effective diffusivity tensor D^* have been obtained only for a handfull of simple models of periodic fluid velocity fields (ANY AT ALL?). We help overcome this limitation by developing novel Fourier methods that provide the mathematical foundation for rigorous computation of D^*. We compute the effective properties for various cellular flows and study the advection dominated, large Péclet number behavior. Our numerical computations are in excellent agreement with known theoretical results. FINISH THIS PARAGRAPH WHEN THE REST OF THE PAPER IS FINISHED.

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

$$\partial_t\phi(t,\boldsymbol{x}) = \boldsymbol{u}(t,\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi(t,\boldsymbol{x}) + \varepsilon\Delta\phi(t,\boldsymbol{x}), \quad \phi(0,\boldsymbol{x}) = \phi_0(\boldsymbol{x}), \quad t>0, \quad \boldsymbol{x}\in\mathbb{R}^d. \tag{2.1}$$

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 periodic fluid flows 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 $t\mapsto t/\eta$ and $x_j\mapsto x_j/\ell$, one finds that ϕ satisfies the advection-diffusion equation in (2.1) with a non-dimensional molecular diffusivity $\varepsilon\mapsto\eta\varepsilon/\ell^2$ and velocity field $\boldsymbol{u}\mapsto\eta\,\boldsymbol{u}/\ell$, where x_j is the $j^{\,\text{th}}$ component of the vector $\boldsymbol{x}$. 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 [60]. Here, we focus on the long time, large scal transport characteristics of equation (2.1) as a function of ε. To this end, we simply take η 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.,

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

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 [87] with an effective diffusivity tensor D^*. In recent decades, methods of homogenization theory [59, 27, 55] 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^* [55]

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

Equations (2.3) follows from the assumption that the initial tracer density ϕ_0 is slowly varying relative to the variations of the velocity field $\boldsymbol{u}$ [59, 28, 55]. This information is incorporated into equation (2.1) by introducing a small dimensionless parameter $\delta\ll 1$ and writing [59, 28, 55]

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

Anticipating that ϕ will have diffusive dynamics as $t\to\infty$, space and time is rescaled according to the standard diffusive relation $\boldsymbol{x}\mapsto\boldsymbol{x}/\delta$ and $t\mapsto t/\delta^2$, and the scalar density according to $\phi^\delta(t,\boldsymbol{x}) = \phi(t/\delta^2,\boldsymbol{x}/\delta)$. The rescaled form of equation (2.1) is given by [55]

$$\partial_t\phi^\delta(t,\boldsymbol{x}) = \delta^{-1}\boldsymbol{u}(t/\delta^2,\boldsymbol{x}/\delta)\cdot\boldsymbol{\nabla}\phi^\delta(t,\boldsymbol{x}) + \varepsilon\Delta\phi^\delta(t,\boldsymbol{x}), \quad \phi(0,\boldsymbol{x}) = \phi_0(\boldsymbol{x}). \tag{2.5}$$

The convergence of ϕ^δ in (2.5) to $\bar\phi$ in (2.3) can be rigorously established in the following sense

$$\lim_{\delta\to 0}\sup_{0\le t\le t_0}\sup_{\boldsymbol{x}\in\mathbb{R}^d}|\phi^\delta(t,\boldsymbol{x})-\bar\phi(t,\boldsymbol{x})|=0, \tag{2.6}$$

for every finite $t_0>0$, provided that ϕ_0 and $\boldsymbol{u}$ obey some mild smoothness and boundedness conditions, and that $\boldsymbol{u}$ satisfies certain averaging conditions described in more detail below [55].

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* [55],

$$\partial_\tau\chi_j(\tau,\boldsymbol{\xi})-\varepsilon\Delta_\xi\chi_j(\tau,\boldsymbol{\xi})-\boldsymbol{u}(\tau,\boldsymbol{\xi})\cdot\boldsymbol{\nabla}_\xi\chi_j(\tau,\boldsymbol{\xi})=u_j(\tau,\boldsymbol{\xi}), \tag{2.7}$$

where the subscript ξ in Δ_ξ and $\boldsymbol{\nabla}_\xi$ indicates that differentiation is with respect to the fast variable $\boldsymbol{\xi}$. More specifically, the components D^*_{jk}, $j,k=1,\dots,d$, of the matrix D^* are given by [59, 27, 55]

$$\mathsf{D}^*_{jk}=\varepsilon\delta_{jk}+\langle u_j\chi_k\rangle, \tag{2.8}$$

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 (2.8) is with respect to the fast variables defined in equation (**??**). 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) $\mathcal{T}\otimes\mathcal{V}$. In the case of a time-dependent fluid velocity field, $\langle\cdot\rangle$ denotes space-time averaging over $\mathcal{T}\otimes\mathcal{V}$. In the special case of a time-independent fluid velocity field, the function χ_j is time-independent and satisfies equation (2.7) with $\partial_\tau\chi_j=0$, and $\langle\cdot\rangle$ in (2.8) denotes spatial averaging over $\mathcal{V}$ [27, 55].

We now discuss conditions that the average of the fluid velocity field must satisfy in order for the homogenization theorem in (2.6) to hold. When the fluid velocity field is mean-zero, then equation (2.6) holds and the effective diffusivity tensor D^* defined in (2.8) is constant [55]. Consequently, only the symmetric part S^* of D^* plays a role in the effective transport equation displayed in (2.9). Now consider the case where the fluid velocity field $\boldsymbol{u}$ is the superposition of a *weak* large-scale mean flow $\boldsymbol{u}_0(t,\boldsymbol{x})$ that varies on large spatial and slow time scales, with a mean-zero periodic flow $\boldsymbol{u}_1(\tau,\boldsymbol{\xi})$ that rapidly fluctuates in space and time, i.e., $\boldsymbol{u}(t,\boldsymbol{x},\tau,\boldsymbol{\xi})=\delta\boldsymbol{u}_0(t,\boldsymbol{x})+\boldsymbol{u}_1(\tau,\boldsymbol{\xi})$ for $\delta\ll 1$ [55]. If $\boldsymbol{u}_0(t,\boldsymbol{x})$ is smooth and bounded, the homegenization theorem for purely periodic velocity fields can be rigorously extended and the effective transport equation in (2.3) is now given by [55]

$$\partial_t\bar\phi(t,\boldsymbol{x})=\boldsymbol{u}_0(t,\boldsymbol{x})\cdot\boldsymbol{\nabla}\bar\phi+\boldsymbol{\nabla}\cdot[\mathsf{D}^*\boldsymbol{\nabla}\bar\phi(t,\boldsymbol{x})],\quad \bar\phi(0,\boldsymbol{x})=\phi_0(\boldsymbol{x}), \tag{2.9}$$

which also includes an advective enhancement in transport by the large-scale mean flow $\boldsymbol{u}_0$ [55]. In this case, the effective diffusivity tensor D^* is completely independent of the mean flow $\boldsymbol{u}_0$ and determined by the same formula in (2.8) and cell problem in (2.7) with $\boldsymbol{u}\to\boldsymbol{u}_1$ [55]. Consequently, D^* is again constant and only the symmetric part S^* of D^* plays a role in the effective transport equation displayed in (2.9).

More generally, one could consider a fluid velocity field that has large-scale structure that varies slowly in space and time relative to rapidly varying spatio-temporal periodic fluctuations, i.e., $\boldsymbol{u}=\boldsymbol{u}(t,\boldsymbol{x},\tau,\boldsymbol{\xi})$ with

$$\boldsymbol{u}(t,\boldsymbol{x},\tau,\boldsymbol{\xi})=\boldsymbol{u}_0(t,\boldsymbol{x})+\boldsymbol{u}_1(t,\boldsymbol{x},\tau,\boldsymbol{\xi}) \tag{2.10}$$

and $\langle\boldsymbol{u}_1\rangle=0$ so that $\boldsymbol{u}_0(t,\boldsymbol{x})=\langle\boldsymbol{u}(t,\boldsymbol{x},\tau,\boldsymbol{\xi})\rangle$. In this case, the average $\langle u_j\chi_k\rangle$ with respect to the fast variables τ and ξ in (2.8) remains a function slow variables t and $\boldsymbol{x}$. Consequently, the components $\mathsf{D}^*_{jk}=\varepsilon\delta_{jk}+\langle u_j\chi_k\rangle$, $j,k=1,\dots,d$, varies slowly in *space and time*, and both the symmetric S^* and antisymmetric A^* parts of D^* play an important role in the effective transport equation [70, 60]. For this reason, here we will develop Stieltjes integral representations for both the symmetric and antisymmetric parts of D^*. As we will demonstrate below, the spectral theory of effective diffusivity is quite flexable and allows for a very large class of fluid velocity fields $\boldsymbol{u}$, even those with non-zero mean which pose considerable technical difficulties [55] in the homogenization theorem leading to equation (2.3). In order to stay in line with the mathematical framework summarized above, we restrict our attention to the more fundamental setting of a mean-zero velocity field and simply indicate the modifications necessary to include more general fluid flows.

In Section 7 we provide a mathematically rigorous formulation of Radon–Stieltjes integral representations for both the symmetric S^* and antisymmetric A^* parts of D^*, as defined in (2.8). This formulation is based on the spectral theorem for *unbounded* self-adjoint operators in Hilbert space. In Section 3, we review the spectral theory of such operators, which arise naturally in the study of effective diffusivity. In Section 4 we give two natural Hilbert space formulations of the effective parameter problem for D^* which lead to the promised integral representations for D^*. In Section **??** we use powerful methods of functional analysis to prove that the two formulations are equivalent and discuss the advantages of each approach.

3. 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 Stone. It is considerably more technical and challanging 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.

Let Φ be a linear operator acting on a Hilbert space $\mathscr{H}$ with sequilinear inner-product $\langle\cdot,\cdot\rangle$ satisfying $\langle a\psi, b\varphi\rangle = \overline{a}\, b\,\langle\psi,\varphi\rangle$ 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 $\|\Phi^*\| = \|\Phi\|$ [77]. Consequently, Φ and its adjoint Φ^* have identical domains,

$$D(\Phi) = D(\Phi^*), \tag{3.1}$$

as they can be taken, without loss of generality [83], to be the entire Hilbert space, $D(\Phi) = D(\Phi^*) = \mathscr{H}$. The operator Φ is said to be *symmetric* if

$$\langle\Phi\psi,\varphi\rangle = \langle\psi,\Phi\varphi\rangle, \ \text{ for all } \ \psi,\varphi\in D(\Phi). \tag{3.2}$$

By definition [77, 85], the two properties (3.1) and (3.2) 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 $\mathscr{H}$ [77]. 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, it is often the case that the domain $D(\Phi)$ can be defined as an *everywhere dense* subset of $\mathscr{H}$ such that Φ is bounded. Moreover, on this domain, Φ can be extended to a *closed* symmetric operator [77, 85]. However, even in this case the domain of the associated adjoint does not always coincide with $D(\Phi)$, and in such circumstances Φ is *not* self-adjoint on $D(\Phi)$. Only for self-adjoint operators does the spectral theorem hold [77, 85].

The spectrum Σ of the self-adjoint operator Φ is real-valued [77, 85]. If Φ is bounded on the Hilbert space $\mathscr{H}$, then its spectral radius equal to its operator norm $\|\Phi\|$ [77], i.e.,

$$\Sigma\subseteq[-\|\Phi\|,\|\Phi\|\,]. \tag{3.3}$$

If Φ is unbounded, its spectrum Σ can be an unbounded subset of, or can even coincide with the set of real numbers $\mathbb{R}$ [85]. We now summarize the spectral theorem for self-adjoint operators. Let $\mathscr{H}_d$ be an everywhere dense subset of the Hilbert space $\mathscr{H}$, on which Φ is self-adjoint. If Φ is bounded then we simply take $\mathscr{H}_d\equiv\mathscr{H}$. 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 $\lim_{\lambda\to\inf\Sigma}Q(\lambda) = 0$ and $\lim_{\lambda\to\sup\Sigma}Q(\lambda) = I$ [85], where I denotes the identity operator on $\mathscr{H}$. 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 $\psi,\varphi\in\mathscr{H}_d$ [85]. 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

$$\mathrm{Re}\;\mu_{\psi\varphi}(\lambda) = \frac{1}{2}\left(\mu_{\psi\varphi}(\lambda)+\overline{\mu}_{\psi\varphi}(\lambda)\right), \quad \mathrm{Im}\;\mu_{\psi\varphi}(\lambda) = \frac{1}{2\,\imath}\left(\mu_{\psi\varphi}(\lambda)-\overline{\mu}_{\psi\varphi}(\lambda)\right), \tag{3.4}$$

where $\mathrm{Re}\,\mu_{\psi\psi}(\lambda) = \mu_{\psi\psi}(\lambda)$ and $\mathrm{Im}\,\mu_{\psi\psi}(\lambda) = 0$. With each of these strictly increasing functions of bounded variation, we associate Stieltjes measures [84, 85, 32]

$$\begin{aligned} \mathrm{d}\mu_{\psi\varphi}(\lambda) &= \mathrm{d}\langle Q(\lambda)\psi,\varphi\rangle, &\qquad \mathrm{dRe}\,\mu_{\psi\varphi}(\lambda) &= \mathrm{dRe}\,\langle Q(\lambda)\psi,\varphi\rangle,\\ \mathrm{d}\mu_{\psi\psi}(\lambda) &= \mathrm{d}\|Q(\lambda)\psi\,\|^2, &\qquad \mathrm{dIm}\,\mu_{\psi\varphi}(\lambda) &= \mathrm{dIm}\,\langle Q(\lambda)\psi,\varphi\rangle, \end{aligned} \tag{3.5}$$

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 [84, 85].

The spectral theorem also provides an operational calculus in Hilbert space which yields powerful integral representations involving the Stieltjes measures displayed in equation (3.5). A summary of the relevent 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 $\psi \in \mathscr{H}_d$ 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 [85]

$$\begin{aligned} \langle F(\Phi)\psi, \varphi\rangle &= \int_{-\infty}^{\infty} \overline{F}(\lambda)\, \mathrm{d}\mu_{\psi\varphi}(\lambda), \qquad \forall\, \psi \in \mathscr{D}(F),\ \varphi \in \mathscr{H}_d, \\ \langle F(\Phi)\psi, G(\Phi)\varphi\rangle &= \int_{-\infty}^{\infty} \overline{F}(\lambda) G(\lambda)\, \mathrm{d}\mu_{\psi\varphi}(\lambda), \quad \forall\, \psi \in \mathscr{D}(F),\ \varphi \in \mathscr{D}(G), \end{aligned} \tag{3.6}$$

where the integration in (3.6) is over the spectrum Σ of Φ [77, 85]. An important property of the self-adjoint operator Φ which will be used later is that its domain $D(\Phi)$ comprises those and only those elements $\psi \in \mathscr{H}_d$ 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

$$\langle \Phi\psi, \varphi\rangle = \int_{-\infty}^{\infty} \lambda\, \mathrm{d}\mu_{\psi\varphi}(\lambda), \qquad \|\Phi\psi\|^2 = \int_{-\infty}^{\infty} \lambda^2\, \mathrm{d}\mu_{\psi\psi}(\lambda), \tag{3.7}$$

where φ is an arbitrary element in $\mathscr{H}_d$ [85]. In fact, this directly determines the one-to-one correspondence between the self-adjoint operator Φ and its resolution of the identity $Q(\lambda)$ [85]. The mass $\mu^0_{\psi\varphi}$ of the measure $\mu_{\psi\varphi}$ satisfies

$$\mu^0_{\psi\varphi} = \int_{-\infty}^{\infty} \mathrm{d}\mu_{\psi\varphi}(\lambda) = \int_{-\infty}^{\infty} \mathrm{d}\langle Q(\lambda)\psi, \varphi\,\rangle = \langle \psi, \varphi\rangle, \qquad |\mu^0_{\psi\varphi}| \le \|\psi\|\,\|\varphi\| < \infty. \tag{3.8}$$

Equation (3.8) demonstrates that the measures in (3.5) are bounded, i.e., have finite mass [85].

Two special cases of (3.6) that will be used later is when $F(\lambda) = G(\lambda)$ and $F(\lambda) = -\imath\lambda G(\lambda)$ with $F(\Phi)\psi,\, G(\Phi)\varphi \in \mathscr{H}$ *real-valued* so that $\langle F(\Phi)\psi, G(\Phi)\varphi\rangle = \langle G(\Phi)\varphi, F(\Phi)\psi\rangle$. In these cases, the identities $\operatorname{Re} z = (z + \overline{z})/2$ and $\operatorname{Im} z = (z - \overline{z})/(2\imath)$ and the linearity properties [85] of Stieltjes-Radon integrals with respect to the functions $\mu_{\psi\varphi}(\lambda)$ and $\overline{\mu}_{\psi\varphi}(\lambda)$ imply that the functional $\langle F(\Phi)\psi, G(\Phi)\varphi\rangle$ has the integral representation displayed in equation (3.6), instead involving the measures $\mathrm{dRe}\,\mu_{\psi\varphi}$ and $\mathrm{dIm}\,\mu_{\psi\varphi}$, respectively.

Equation (3.6) can be generalized, holding with suitable notational changes, for *maximal normal operators* [85]. Such a normal operator $\mathbf{N}$ with domain $D(\mathbf{N})$ 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 $\mathbb{C}$ [85]. A special case of a normal operator, which arises naturally in the spectral theory of effective diffusivity discussed in Section **??**, is a *skew-adjoint* operator, which satisfies $\mathbf{N}^* = -\mathbf{N}$ and can be decomposed as $\mathbf{N} = \imath\Phi_2$ where Φ_2 is self-adjoint. Since Φ_2 is self-adjoint having purely real spectrum, it is clear that the skew-adjoint operator $\mathbf{N} = \imath\Phi_2$ has purely imaginary spectrum [85]. Since an operator is self-adjoint if and only if it is a maximal normal operator [85], we can simply focus on the spectral characterization of the self-adjoint operator $\Phi_2 = -\imath\mathbf{N}$.

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. We demonstrate later that the operator ∂_t plays a central role in the spectral theory of effective diffusivity for time-dependent flows. 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

$$\varphi_n(t) = \beta \sin(n\pi t/T), \quad \beta = \sqrt{2/T}, \qquad \langle \varphi_n, \varphi_m\rangle_2 = \delta_{nm}, \quad n, m \in \mathbb{N}, \tag{3.9}$$

where $\langle\cdot,\cdot\rangle_2$ denotes the sesquilinear $L^2(\mathcal{T})$-inner-product. Since $\partial_t\varphi_n = (n\pi\beta/T)\cos(n\pi t/T)$ and $\|\partial_t\varphi_n\|^2 = (n\pi/T)^2$, 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 [77, 85]. Consider the class $\mathscr{A}_\mathcal{T}$ of all functions $\psi \in L^2(\mathcal{T})$ such that $\psi(t)$ is *absolutely continuous* [78] on the interval $\mathcal{T}$ and has a derivative $\psi'(t)$ belonging to $L^2(\mathcal{T})$, i.e. [85, 78]

$$\mathscr{A}_\mathcal{T} = \left\{ \psi \in L^2(\mathcal{T}) \;\Big|\; \psi(t) = c + \int_0^t g(s)ds, \quad g \in L^2(\mathcal{T}) \right\}, \tag{3.10}$$

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 (3.10) with $\int_0^T g(s)ds = 0$. In order to help clairify the ideas that were discussed above in terms of the 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 (3.10) with $c = 0$ and $\int_0^T g(s)ds = 0$. More concisely,

$$\tilde{\mathscr{A}_\mathcal{T}} = \{\psi \in \mathscr{A}_\mathcal{T} \,|\, \psi(0) = \psi(T)\}, \qquad \hat{\mathscr{A}_\mathcal{T}} = \{\psi \in \mathscr{A}_\mathcal{T} \,|\, \psi(0) = \psi(T) = 0\}. \tag{3.11}$$

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 $L^2(\mathcal{T})$ [85]. 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 adjoint $\hat{B}^* \equiv B$, and the operator $\tilde{B}$ is a *self-adjoint* extension of $\hat{B}$ [85]. 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.

In Section 4 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 (2.8) and (2.7), involving self-adjoint operators on appropriate Hilbert spaces. In Section 7.3 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 (3.7). FINISH THIS PARAGRAPH AFTER SECTION Section 4 IS WRITTEN.

4. Hilbert spaces, resolvents, and integral representations of the effective diffusivity. In this section we formulate the spectral theory of effective diffusivity. In Section 4.1 we provide two abstract Hilbert space formulations of the effective parameter problem for advective diffusion as well as resolvent formulas for the curl-free field $\boldsymbol{\nabla}\chi_j$ and the scalar field χ_j, involving self-adjoint operators with domains defined as everywhere dense subsets of the associated Hilbert space. These resolvent formulas, in turn, lead to Stieltjes-Radon integral representations for the symmetric and antisymmetric parts of the effective diffusivity tensor D^*, discussed in Section 7.

4.1. Hilbert spaces, resolvents, and isometric correspondences. Consider the following sets $\mathcal{T} = [0, T]$ and $\mathcal{V} = \otimes_{j=1}^d [0, \ell]$ which define the space-time period cell $\mathcal{T} \otimes \mathcal{V}$ associated with the periodic fluid velocity field $\boldsymbol{u}(t, \boldsymbol{x})$ in (2.2). Now consider the Hilbert spaces $\mathscr{H}_\mathcal{T}$ and $\mathscr{H}_\mathcal{V}$ as well as their direct product $\mathscr{H}_{\mathcal{T}\mathcal{V}}$, over the complex field $\mathbb{C}$, defined by

$$\mathscr{H}_{\mathcal{T}\mathcal{V}} = \mathscr{H}_\mathcal{T} \otimes \mathscr{H}_\mathcal{V}, \quad \mathscr{H}_\mathcal{T} = \big\{\psi \in L^2(\mathcal{T}) \,|\, \psi(t) = \psi(t+T)\big\}, \quad \mathscr{H}_\mathcal{V} = \big\{\psi \in L^2(\mathcal{V}) \,|\, \psi(\boldsymbol{x}) = \psi(\boldsymbol{x} + \ell\boldsymbol{e}_j)\big\}, \tag{4.1}$$

for all $j = 1, \ldots, d$. In equation (3.11) we defined the space $\tilde{\mathscr{A}_\mathcal{T}}$ of absolutely continuous $\mathcal{T}$-periodic functions, which is an everywhere dense subset of $\mathscr{H}_\mathcal{T}$. Now define the Sobolev space $\mathscr{H}_\mathcal{V}^1 \subset \mathscr{H}_\mathcal{V}$,

$$\mathscr{H}_\mathcal{V}^1 = \big\{\psi \in \mathscr{H}_\mathcal{V} \mid \langle|\boldsymbol{\nabla}\psi|^2\rangle_\mathcal{V} < \infty\big\}, \tag{4.2}$$

which is also a Hilbert space [31], 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

$$\mathscr{H} = \big\{\psi \in \mathscr{H}_\mathcal{T} \otimes \mathscr{H}_\mathcal{V}^1 \mid \langle\psi\rangle = 0\big\}, \qquad \mathscr{F} = \big\{\psi \in \tilde{\mathscr{A}_\mathcal{T}} \otimes \mathscr{H}_\mathcal{V}^1 \mid \langle\psi\rangle = 0\big\}. \tag{4.3}$$

Here, $\langle\cdot\rangle$ denotes space-time averaging over the period cell $\mathcal{T}\times\mathcal{V}$. Recalling that $\boldsymbol{\psi}\cdot\boldsymbol{\varphi}=\boldsymbol{\psi}^\dagger\boldsymbol{\varphi}$, denote by $\|\cdot\|_1$ the norm induced by the the sesquilinear inner-product $\langle\cdot,\cdot\rangle_1$ associated with the Hilbert space $\mathscr{H}$, defined by $\langle\psi,\varphi\rangle_1=\langle\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\varphi\rangle$ with $\langle\varphi,\psi\rangle_1=\overline{\langle\psi,\varphi\rangle}_1$. We stress that $\psi\in\mathscr{F}$ implies $\|\partial_t\psi\|_1<\infty$ and $\|\psi\|_1<\infty$. In the case of a time-independent velocity field $\boldsymbol{u}(\boldsymbol{x})$ we set $\tilde{\mathscr{A}_{\mathcal{T}}}=\emptyset$ in (4.3), so that $\psi\in\mathscr{F}$ implies $\psi\in\mathscr{H}^1_{\mathcal{V}}$ with $\langle\psi\rangle_{\mathcal{V}}=0$.

We now use the mathematical 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^*, with components defined in equation (2.8). Moreover, we transform the cell problem in equation (2.7) into a resolvent formula for the function χ_j, involving an operator which is self-adjoint on $\mathscr{F}$. In Section 7, we demonstrate that these results lead to Stieltjes integral representations for both S^* and A^*.

In terms of the $\mathscr{H}$-inner-product $\langle\cdot,\cdot\rangle_1$, the components S^*_{jk} and A^*_{jk}, $j,k=1,\ldots,d$, of S^* and A^* are given by the following functional formulas [70],

$$\mathsf{S}^*_{jk}=\varepsilon(\delta_{jk}+\langle\chi_j,\chi_k\rangle_1),\qquad \mathsf{A}^*_{jk}=\langle A\chi_j,\chi_k\rangle_1,\quad A=(-\Delta)^{-1}(\partial_t-\boldsymbol{u}\cdot\boldsymbol{\nabla}). \tag{4.4}$$

We now discuss the symmetry properties of the matrices S^* and A^* as defined by equation (4.4). Since the scalar field χ_j is *real-valued* for all $j=1,\ldots,d$ and the operator A maps real-valued fields to real-valued fields, we have

$$\langle\chi_j,\chi_k\rangle_1=\langle\chi_k,\chi_j\rangle_1,\quad \langle A\chi_j,\chi_k\rangle_1=\langle\chi_k,A\chi_j\rangle_1. \tag{4.5}$$

The first formula in (4.5) clearly implies that $\mathsf{S}^*_{jk}=\mathsf{S}^*_{kj}$, hence the matrix S^* is symmetric. We show in Section A.1 that A is an antisymmetric operator on the function space $\mathscr{F}$. Consequently, we have $\mathsf{A}^*_{jk}=\langle A\chi_j,\chi_k\rangle_1=-\langle\chi_j,A\chi_k\rangle_1=-\langle A\chi_k,\chi_j\rangle_1=-\mathsf{A}^*_{kj}$, which implies that the matrix A^* is indeed skew-symmetric.

The formulas for S^*_{jk} and A^*_{jk} in equation (4.4) follow [70] from the formula $\mathsf{D}^*_{jk}=\varepsilon\delta_{jk}+\langle u_j\chi_k\rangle$ in equation (2.8) and the cell problem $u_j=-\varepsilon\Delta\chi_j+(\partial_t-\boldsymbol{u}\cdot\boldsymbol{\nabla})\chi_j$ in (2.7). More specifically, since $\mathcal{V}$ is a bounded domain, the operator $(-\Delta)^{-1}$ is a bounded linear operator on the Hilbert space $L^2(\mathcal{V})$ [83], hence on $\mathscr{H}^1_{\mathcal{V}}$ as $\mathscr{H}^1_{\mathcal{V}}\subset L^2(\mathcal{V})$. For u_j and χ_j in suitable function spaces discussed in detail below, we may consequently write

$$\langle u_j\chi_k\rangle=\langle[\Delta\Delta^{-1}u_j]\,\chi_k\rangle=-\langle\boldsymbol{\nabla}\Delta^{-1}u_j\cdot\boldsymbol{\nabla}\chi_k\rangle=-\langle\Delta^{-1}u_j,\chi_k\rangle_1=\varepsilon\langle\chi_j,\chi_k\rangle_1+\langle A\chi_j,\chi_k\rangle_1, \tag{4.6}$$

where the periodicity of u_j and χ_k was used in the second equality and the cell problem was used in the final equality.

Applying the operator $(-\Delta)^{-1}$ to both sides of the cell problem in equation (2.7) yields [70] the following resolvent formula for the scalar field χ_j involving the operator A defined in equation (4.4)

$$\chi_j=(\varepsilon+A)^{-1}g_j,\qquad g_j=(-\Delta)^{-1}u_j. \tag{4.7}$$

From equations (4.4) and (4.7) we have the following functional formulas for S^*_{jk} and A^*_{jk}, involving the antisymmetric operator A

$$\mathsf{S}^*_{jk}=\varepsilon\left(\delta_{jk}+\langle(\varepsilon+A)^{-1}g_j,(\varepsilon+A)^{-1}g_k\rangle_1\right),\quad \mathsf{A}^*_{jk}=\langle A(\varepsilon+A)^{-1}g_j,(\varepsilon+A)^{-1}g_k\rangle_1. \tag{4.8}$$

In Section 7, we use the functional formulas displayed in equation (4.8), the spectral properties of the operator A, and the spectral theorem in (3.6) to provide Stieltjes integral representations for S^* and A^*.

We mentoned above that Stieltjes integral representations for the symmetric S^* and antisymmetric A^* parts of the effective diffusivity tensor D^* can be rigorously established for a large class of fluid velocity fields $\boldsymbol{u}$. Indeed the mathematical framework that we formulate below holds when the components u_j of $\boldsymbol{u}$ and the functions χ_j, $j=1,\ldots,d$, satisfy the following conditions

$$u_j\in\tilde{\mathscr{A}_{\mathcal{T}}}\otimes\mathscr{H}_{\mathcal{V}},\quad \chi_j\in\tilde{\mathscr{A}_{\mathcal{T}}}\otimes\mathscr{H}^1_{\mathcal{V}}. \tag{4.9}$$

In particular, it is *not* necessary that $\langle u_j\rangle=0$ nor $\langle\chi_j\rangle=0$. We now discuss this in more detail. In equation (4.6) we wrote the $\mathscr{H}_{\mathcal{T}\mathcal{V}}$-inner-product $\langle u_j\chi_k\rangle$ of the functions u_j and χ_k as $\langle[\Delta\Delta^{-1}u_j]\,\chi_k\rangle$, which assumes that this quantity is bounded. This holds when $\chi_k(t,\cdot)\in\mathscr{H}_{\mathcal{V}}$ and $u_j(t,\cdot)\in C^1(\overline{\mathcal{V}})$ for all $t\in\mathcal{T}$, as in this case we have $\Delta^{-1}u_j(t,\cdot) \in C^2(\mathcal{V})$ [61], where $\overline{\mathcal{V}}$ is the closure of $\mathcal{V}$ and $C^n(\mathcal{V})$ is the space of continuously differentiable functions on $\mathcal{V}$ of order n. However, after integrating by parts we wrote $\langle u_j\chi_k\rangle$ as $-\langle\Delta^{-1}u_j,\chi_k\rangle_1$, which is bounded when $\chi_k(t,\cdot) \in \mathscr{H}^1_{\mathcal{V}}$ and $u_j(t,\cdot) \in L^1(\mathcal{V})$ and bounded on $\mathcal{V}$, as in this case $\Delta^{-1}u_j(t,\cdot) \in C^1(\overline{\mathcal{V}})$ [61]. However, inserting the cell problem into this expression we obtained equation (4.4) which, due to the presence of the operator A, is bounded for $\chi_j \in \tilde{\mathscr{A}_{\mathcal{T}}} \otimes \mathscr{H}^1_{\mathcal{V}}$. Finally, writing (4.4) as in (4.8) and recalling the spectral theorem in (3.6), we will show in Section 7 that the promised Stieltjes integral representations of the functionals in (4.8) hold when the scalar fields u_j and χ_j satisfy equation (4.9). Consequently, given a fluid velocity field $\boldsymbol{u}$ with components u_j satisfying the first formula in equation (4.9), if the cell problem in (2.7) has a solution χ_j satisfying the second formula in equation (4.9) such that equation (2.6) holds in some generalized, weak sense, then the integral representaions for S^* and A^* discussed in Section 7 rigorously hold. This framework allows for the fluid velocity field $\boldsymbol{u}$ to have a mean *everywhere bounded* $\langle\boldsymbol{u}\rangle$ that is slowly varying in *everywhere bounded* mean For concretness, we develop the theory for the case of mean-zero scalar fields u_j and χ_j.

We now provide an alternate formulation of the effective parameter problem [4, 5] which provides analogous formulas to those in equations (4.4) and (4.7) involving the *curl-free* field $\boldsymbol{\nabla}\chi_j$ displayed in equation (2.7). Towards this goal, consider the Hilbert spaces given by that in equation (4.1), except over the d-dimensional complex field $\mathbb{C}^d$,

$$\mathcal{H}_{\mathcal{T}\mathcal{V}} = \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}, \quad \mathcal{H}_{\mathcal{T}} = \otimes_{j=1}^d \mathscr{H}_{\mathcal{T}}, \quad \mathcal{H}_{\mathcal{V}} = \otimes_{j=1}^d \mathscr{H}_{\mathcal{V}}. \tag{4.10}$$

By the Helmholtz theorem [54, 10], the Hilbert space $\mathcal{H}_{\mathcal{V}}$ can be decomposed, $\mathcal{H}_{\mathcal{V}} = \mathcal{H}_W \oplus \mathcal{H}_{\bullet} \oplus \mathcal{H}_0$, into mutually orthogonal subspaces of curl-free $\mathcal{H}_W$, divergence-free $\mathcal{H}_{\bullet}$, and constant $\mathcal{H}_0$ vector fields, with associated orthogonal projectors $\Gamma_W = \boldsymbol{\nabla}(\Delta^{-1})\boldsymbol{\nabla\cdot}$, $\Gamma_{\bullet} = -\boldsymbol{\nabla}W(\boldsymbol{\Delta}^{-1})\boldsymbol{\nabla}W$, and $\Gamma_0 = \langle\cdot\rangle$, respectively, satisfying $I = \Gamma_W + \Gamma_{\bullet} + \Gamma_0$ [27, 63], where 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 (2.7), we will find particular use of the Hilbert space $\mathcal{H}_W$, which we define by

$$\mathcal{H}_W = \{\boldsymbol{\psi} \in \mathcal{H}_{\mathcal{V}} \mid \Gamma\boldsymbol{\psi} = \boldsymbol{\psi}\}, \quad \Gamma = \boldsymbol{\nabla}(\Delta^{-1})\boldsymbol{\nabla\cdot}, \tag{4.11}$$

where we have denoted Γ_W by Γ for notational simplicity. Analogous to equation (4.3), we define the Hilbert space $\mathcal{H}$ and its everywhere dense subset $\mathcal{F}$,

$$\mathcal{H} = \{\boldsymbol{\psi} \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_W \mid \langle\boldsymbol{\psi}\rangle = 0\}, \qquad \mathcal{F} = \{\boldsymbol{\psi} \in \tilde{\mathcal{A}}_{\mathcal{T}} \otimes \mathcal{H}_W \mid \langle\boldsymbol{\psi}\rangle = 0\}, \tag{4.12}$$

where we have defined $\tilde{\mathcal{A}}_{\mathcal{T}} = \otimes_{j=1}^d \tilde{\mathscr{A}_{\mathcal{T}}}$ which is an everywhere dense subset of the Hilbert space $\mathcal{H}_{\mathcal{T}}$. 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 $\langle\boldsymbol{\psi},\boldsymbol{\varphi}\rangle = \overline{\langle\boldsymbol{\varphi},\boldsymbol{\psi}\rangle}$.

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

$$\boldsymbol{u} = \boldsymbol{\nabla}\cdot\mathsf{H}, \qquad \mathsf{H}^T = -\mathsf{H}, \tag{4.13}$$

where H^T denotes transposition of the matrix H. Using this representation of the fluid velocity field, 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 in terms of the $\mathcal{H}$-inner-product $\langle\cdot,\cdot\rangle$ by the following functional formulas [4, 5]

$$\mathsf{S}^*_{jk} = \varepsilon(\delta_{jk} + \langle\boldsymbol{\nabla}\chi_j,\boldsymbol{\nabla}\chi_k\rangle), \qquad \mathsf{A}^*_{jk} = \langle\mathbf{A}\boldsymbol{\nabla}\chi_j,\boldsymbol{\nabla}\chi_k\rangle, \qquad \mathbf{A} = \Gamma[\mathsf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}]\Gamma, \quad \mathbf{T} = \partial_t\mathbf{I}. \tag{4.14}$$

Here, $\mathbf{T} = \mathrm{diag}(\partial_t,\ldots,\partial_t)$ operates component-wise on d-dimensional vector fields, the inverse of the vector Laplacian $\boldsymbol{\Delta}$ is denoted by $\boldsymbol{\Delta}^{-1} = \mathrm{diag}(\Delta^{-1},\ldots,\Delta^{-1})$, where Δ^{-1} is based on convolution with the Green's function for the Laplacian Δ on $\mathcal{V}$ [83].

The formulas in equation (4.14) are obtainded by casting the cell problem in (2.7) into a form which parallels the effective parameter problem for transport in composite materials [4, 5]. This allows one to bring to bear well developed mathematical techniques of the analytic continuation method for representing transport in composites [36, 63]. This method provides Stieltjes integral representations for the effective transport coefficients of composite media, involving a spectral measure of a self-adjoint operator which depends only on the composite geometry [36, 66, 63].

Towards this goal, we now transform the cell problem in (2.7) into a divergence equation [27] which immediately yields equation (4.14) and readily leads to a resolvent formula for the curl-free vector field $\boldsymbol{\nabla}\chi_j$, analogous to that for the scalar field χ_j displayed in (4.7). Using the representation of the fluid velocity field given in (4.13), the advection-diffusion equation in (2.1) can be written as a diffusion equation, $\partial_t\phi = \boldsymbol{\nabla}\cdot[\mathsf{D}\boldsymbol{\nabla}\phi]$, where $\mathsf{D}(t,\boldsymbol{x}) = \varepsilon\mathsf{I} + \mathsf{H}(t,\boldsymbol{x})$ can be viewed as a local diffusivity tensor. The cell problem in (2.7) can also be written as the following diffusion equation [27]

$$\partial_t\chi_j = \boldsymbol{\nabla}\cdot[\mathsf{D}(\boldsymbol{\nabla}\chi_j + \boldsymbol{e}_j)], \quad \langle\boldsymbol{\nabla}\chi_k\rangle = 0, \qquad \mathsf{D} = \varepsilon\mathsf{I} + \mathsf{H}. \tag{4.15}$$

Due to the skew-symmetry of the matrix H, we have the identity $[\boldsymbol{\nabla}\cdot\mathsf{H}\,]\cdot\boldsymbol{\nabla}\chi_j = \boldsymbol{\nabla}\cdot[\mathsf{H}\boldsymbol{\nabla}\chi_j]$. Now, writing $\partial_t\chi_j = \Delta\Delta^{-1}\partial_t\chi_j = \boldsymbol{\nabla}\cdot(\boldsymbol{\Delta}^{-1}\mathbf{T})\boldsymbol{\nabla}\chi_j$ and $\boldsymbol{E}_j = \boldsymbol{\nabla}\chi_j + \boldsymbol{e}_j$, equation (4.15) can be written in divergence form [27],

$$\boldsymbol{\nabla}\cdot[\boldsymbol{\sigma}\boldsymbol{E}_j] = 0, \quad \langle\boldsymbol{E}_j\rangle = \boldsymbol{e}_j, \qquad \boldsymbol{\sigma} = \varepsilon\mathsf{I} + \mathsf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}, \tag{4.16}$$

where we have written $\boldsymbol{\nabla}(\Delta^{-1})\partial_t = \boldsymbol{\Delta}^{-1}\mathbf{T}\boldsymbol{\nabla}$. In terms of the curl-free vector field $\boldsymbol{\nabla}\chi_j$, equation (4.16) is given by $\boldsymbol{\nabla}\cdot[\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_j] = -u_j$. Equation (4.14) now follows from the formula $\mathsf{D}^*_{jk} = \varepsilon\delta_{jk} + \langle u_j\chi_k\rangle$ in equation (2.8), yielding

$$\langle u_j\chi_k\rangle = -\langle[\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_j]\,\chi_k\rangle = \langle\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle = \varepsilon\langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle + \langle\Gamma[\mathsf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}]\Gamma\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle, \tag{4.17}$$

where we have used the periodicity of χ_k and H in the second equality and the final equality follows from the property $\Gamma\boldsymbol{\nabla}\chi_j = \boldsymbol{\nabla}\chi_j$ of the *self-adjoint* operator Γ on $\mathcal{H}$, defined in (4.11).

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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 $\mathcal{H}_W$ and $\mathscr{H}^1_\mathcal{V}$ defined in equations (4.11) and (4.2), 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 $\Delta^{-1}\Delta f = f$ [83], which implies that $\Gamma\boldsymbol{\nabla}f = \boldsymbol{\nabla}f$ 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 $\boldsymbol{\nabla}f\in\mathcal{H}_W$. Conversely, $\boldsymbol{\psi}\in\mathcal{H}_W$ implies that $\boldsymbol{\psi} = \Gamma\boldsymbol{\psi} = \boldsymbol{\nabla}f$, 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 $\Gamma\boldsymbol{\psi} = \boldsymbol{\psi}$ implies that $\|f_1 - f_2\|_1 = \|\boldsymbol{\psi} - \boldsymbol{\psi}\| = 0$. Consequently, for every $\boldsymbol{\psi}\in\mathcal{H}_W$ 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 $\mathcal{H}_W$ are in one-to-one isometric correspondence, which we denote by $\mathscr{H}^1_\mathcal{V}\sim\mathcal{H}_W$. This, in turn, implies that $\mathscr{F}\sim\mathcal{F}$. IS $\tilde{\mathscr{A}}_\mathcal{T}\sim\tilde{\mathcal{A}}_\mathcal{T}$?

We are primarily concerned with fluid velocity fields $\boldsymbol{u}$ such that $0 < \mathsf{D}^*_{kk} < \infty$ for all $0 < \varepsilon < \infty$. Consequently, in view of equation (4.14), we require that the (weakly) curl-free vector field $\boldsymbol{\nabla}\chi_k$ satisfies $\boldsymbol{\nabla}\chi_k \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_W \subset \mathcal{H}_{\mathcal{TV}}$, so that it is bounded in the norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{TV}}$-inner-product [32], $\|\boldsymbol{\nabla}\chi_k\| < \infty$. Defining the (weakly) divergence-free vector field $\boldsymbol{J}_k = \boldsymbol{\sigma}\boldsymbol{e}_k$ in (5.10) as a member of a subset of $\mathcal{H}_{\mathcal{TV}}$ is technically difficult, due to the *unboundedness* of the linear operator $\boldsymbol{\sigma} = \mathsf{D} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ on this space. We now explore the properties of this operator in more detail.

Since $\mathcal{V}$ is a bounded domain, (Δ^{-1}) is a compact operator [83] on the Hilbert space $L^2(\mathcal{V})$. Hence $(\boldsymbol{\Delta}^{-1})$ is a compact operator on the Hilbert space $\mathcal{H}_{\mathcal{V}}$, and is consequently bounded in the operator norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{TV}}$-inner-product [77, 85, 83], when considered as an operator on $\mathcal{H}_{\mathcal{TV}}$. We have already assumed for the convergence $\phi^\delta \to \bar{\phi}$, as $\delta \to 0$, that the flow matrix $\mathsf{H}(t,\boldsymbol{x})$ is periodic on $\mathcal{T} \times \mathcal{V}$. We will also assume that it is (component-wise) mean-zero and bounded in operator norm, and that its component-wise time derivative $\mathbf{T}\mathsf{H}$ is also bounded on $\mathcal{H}_{\mathcal{TV}}$

$$\langle \mathsf{H} \rangle = 0, \quad \|\mathsf{H}\| < \infty, \quad \|\mathbf{T}\mathsf{H}\| < \infty. \tag{4.18}$$

This implies that $\mathsf{D} = \varepsilon\mathsf{I} + \mathsf{H}$ is also bounded for all $0 < \varepsilon < \infty$. Consequently, in the case of a time-independent velocity field $\boldsymbol{u}$, where $\boldsymbol{\sigma} = \mathsf{D}$, the linear operator $\boldsymbol{\sigma}$ is bounded. This and $\|\boldsymbol{\nabla}\chi_k\| < \infty$ implies that $\boldsymbol{J}_k \in \mathcal{H}_\bullet$. Therefore, in the case of a time-dependent velocity field, under the assumptions of (6.3), the unboundedness of $\boldsymbol{\sigma} = \mathsf{D} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ on $\mathcal{H}_{\mathcal{TV}}$ is due to the unboundedness of $\mathbf{T}$ on $\mathcal{H}_{\mathcal{T}}$.

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

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

$$\boldsymbol{u} = \boldsymbol{\nabla}\cdot\mathsf{H}, \qquad \mathsf{H}^T = -\mathsf{H}, \tag{5.1}$$

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

$$\partial_t\phi = \boldsymbol{\nabla}\cdot\mathsf{D}\boldsymbol{\nabla}\phi, \quad \phi(0,\boldsymbol{x}) = \phi_0(\boldsymbol{x}), \qquad \mathsf{D} = \varepsilon\mathsf{I} + \mathsf{H}, \tag{5.2}$$

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

$$\varepsilon_{jk} = \varepsilon\delta_{jk} + \mathsf{H}_{jk}, \quad j,k = 1,\dots,d. \tag{5.3}$$

We denote by I the identity operator on all linear spaces in question.

We are interested in the dynamics of ϕ in (**??**) for *large* length and time scales, and when the initial density ϕ_0 is slowly varying relative to the velocity field $\boldsymbol{u}$. Anticipating that ϕ will have diffusive dynamics, we re-scale space and time by $\boldsymbol{x} \to \boldsymbol{x}/\delta$ and $t \to t/\delta^2$, respectively. For periodic diffusivity coefficients in (**??**) which are uniformly elliptic but not necessarily symmetric, it can be shown [27] that, as $\delta \to 0$, the associated solution $\phi^\delta(t,\boldsymbol{x})$ of (**??**) converges to $\bar{\phi}(t,\boldsymbol{x})$, which satisfies the following diffusion equation involving a (constant) effective diffusivity tensor D^*

$$\partial_t\bar{\phi} = \boldsymbol{\nabla}\cdot\mathsf{D}^*\boldsymbol{\nabla}\bar{\phi}, \quad \bar{\phi}(0,\boldsymbol{x}) = \phi_0(\boldsymbol{x}). \tag{5.4}$$

The components $\mathsf{D}^*_{jk} = \mathsf{D}^*\boldsymbol{e}_j\cdot\boldsymbol{e}_k$ of the effective tensor D^* are given by $\mathsf{D}^*_{jk} = \varepsilon\delta_{jk} + \langle u_j\chi_k\rangle$. For each standard basis vector $\boldsymbol{e}_k$, $k = 1,\dots,d$, the function $\chi_k = \chi_k(t,\boldsymbol{x}\,;\boldsymbol{e}_k)$ satisfies [27] the cell problem

$$\partial_t\chi_k = \boldsymbol{\nabla}\cdot\mathsf{D}(\boldsymbol{\nabla}\chi_k + \boldsymbol{e}_k), \quad \langle\boldsymbol{\nabla}\chi_k\rangle = 0. \tag{5.5}$$

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

$$\mathsf{D}^* = \mathsf{S}^* + \mathsf{A}^*, \qquad \mathsf{S}^* = \frac{1}{2}\left(\mathsf{D}^* + [\mathsf{D}^*]^T\right), \quad \mathsf{A}^* = \frac{1}{2}\left(\mathsf{D}^* - [\mathsf{D}^*]^T\right). \tag{5.6}$$

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

$$\mathsf{S}^*_{jk} = \varepsilon(\delta_{jk} + \langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle), \qquad \mathsf{A}^*_{jk} = \langle\mathbf{S}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle, \qquad \mathbf{S} = \mathsf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}, \quad \mathbf{T} = \partial_t\mathsf{I}, \tag{5.7}$$

where $\boldsymbol{\psi}\cdot\boldsymbol{\varphi}=\boldsymbol{\psi}^\dagger\boldsymbol{\varphi}$ denotes the $\ell^2(\mathbb{C}^N)$ inner-product and $\dagger$ is the operation of complex-conjugate-transpose. Here, $\mathbf{T}=\mathrm{diag}(\partial_t,\ldots,\partial_t)$ operates component-wise on vector fields, $\boldsymbol{\Delta}^{-1}=\mathrm{diag}(\Delta^{-1},\ldots,\Delta^{-1})$ is the inverse of the vector Laplacian, and the inverse operation Δ^{-1} is based on convolution with the Green's function for the Laplacian Δ on $\mathcal{V}$ [83]. We stress that, while the effective diffusivity tensor D^* is not symmetric in general, only its symmetric part appears in the homogenized equation [59] in (2.3).

Due to the fact that the vector field $\boldsymbol{\nabla}\chi_j$ is *real-valued*, we have that $\langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle=\langle\boldsymbol{\nabla}\chi_k\cdot\boldsymbol{\nabla}\chi_j\rangle$. From equation (4.14) this clearly implies that the tensor D^* is symmetric, $\mathsf{S}^*_{jk}=\mathsf{S}^*_{kj}$. Moreover, equation (4.14) demonstrates that the effective transport of the tracer ϕ in the principle directions $\boldsymbol{e}_k$, $k=1,\ldots,d$, is always *enhanced* by the presence of an incompressible velocity field, $\mathsf{D}^*_{kk}=\mathsf{S}^*_{kk}\geq\varepsilon$. The equality $\mathsf{D}^*_{kk}=\mathsf{S}^*_{kk}$ follows from the skew-symmetry of A^*, so that $\mathsf{A}^*_{kj}=-\mathsf{A}^*_{jk}$ and $\mathsf{A}^*_{kk}=0$. This, in turn, follows from the skew-symmetry of the operator $\mathbf{S}$ (see Section A.1), $\mathsf{A}^*_{jk}=\langle\mathbf{S}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle=-\langle\mathbf{S}\boldsymbol{\nabla}\chi_k\cdot\boldsymbol{\nabla}\chi_j\rangle=-\mathsf{A}^*_{kj}$ and

$$\mathsf{A}^*_{kk}=\langle\mathbf{S}\boldsymbol{\nabla}\chi_k\cdot\boldsymbol{\nabla}\chi_k\rangle=-\langle\mathbf{S}\boldsymbol{\nabla}\chi_k\cdot\boldsymbol{\nabla}\chi_k\rangle=0. \tag{5.8}$$

In Section 6 we discuss the properties of the linear operator $\mathbf{S}$ and the vector field $\boldsymbol{\nabla}\chi_j$ in more detail.

We now recast equations (4.15) and (4.14) into a form which parallels the effective parameter problem for transport in composites. This allows us to bring to bear on the effective parameter problem for advective diffusion, the well developed mathematical techniques of the analytic continuation method for characterizing effective transport in composite media [36, 63]. This method gives a Hilbert space formulation of the effective parameter problem and provides an integral representation for the effective transport coefficients of composites, involving a *spectral measure* of a self-adjoint operator which depends only on the composite geometry [36, 66, 63]. Here we establish a correspondence between this effective parameter problem and that for enhanced diffusive transport by advective velocity fields. In Section 6, we formulate the Hilbert space framework associated with advective diffusion, and employ it to obtain a resolvent representation of the vector field $\boldsymbol{\nabla}\chi_k$ in (4.15). In Section 7 we utilize this mathematical framework to obtain integral representations for D^* and A^*, involving a spectral measure which depends only on the fluid velocity field $\boldsymbol{u}$.

Toward this goal, we recast the first formula in equation (4.15) in a more suggestive, divergence form. Using the notation from equation (4.14) we write

$$\boldsymbol{\nabla}(\Delta^{-1})\partial_t=\boldsymbol{\Delta}^{-1}\mathbf{T}\boldsymbol{\nabla}, \tag{5.9}$$

so that [27] $\partial_t\chi_k=\Delta\Delta^{-1}\partial_t\chi_k=\boldsymbol{\nabla}\cdot(\boldsymbol{\Delta}^{-1}\mathbf{T})\boldsymbol{\nabla}\chi_k$. Define the vector field $\boldsymbol{e}_k=\boldsymbol{\nabla}\chi_k+\boldsymbol{e}_k$ and the operator $\boldsymbol{\sigma}=\mathsf{D}-(\boldsymbol{\Delta}^{-1})\mathbf{T}=\varepsilon\mathsf{I}+\mathbf{S}$, where $\boldsymbol{\sigma}=\mathsf{D}=\varepsilon\mathsf{I}+\mathsf{H}$ in the case of steady fluid velocity fields. With these definitions, equation (4.15) may be written as $\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\boldsymbol{e}_k=0$, $\langle\boldsymbol{e}_k\rangle=\boldsymbol{e}_k$, which is equivalent to

$$\boldsymbol{\nabla}\cdot\boldsymbol{J}_k=0,\quad \boldsymbol{\nabla}W\boldsymbol{e}_k=0,\quad \boldsymbol{J}_k=\boldsymbol{\sigma}\boldsymbol{e}_k,\quad \langle\boldsymbol{e}_k\rangle=\boldsymbol{e}_k,\qquad \boldsymbol{\sigma}=\varepsilon\mathsf{I}+\mathbf{S}. \tag{5.10}$$

The formulas in (5.10) are precisely the electrostatic version of Maxwell's equations for a conductive medium [36], 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, the effective conductivity tensor $\boldsymbol{\sigma}^*$ is defined as

$$\langle\boldsymbol{J}_k\rangle=\boldsymbol{\sigma}^*\langle\boldsymbol{e}_k\rangle. \tag{5.11}$$

The linear constitutive relation $\boldsymbol{J}_k=\boldsymbol{\sigma}\boldsymbol{e}_k$ in (5.10) relates the local intensity and flux, while that in (5.11) relates the mean intensity and flux. Due to the skew-symmetry of $\mathbf{S}$, the intensity-flux relationship in (5.10) is similar to that of a Hall medium [44].

For the (constant) tensors D^* and $\boldsymbol{\sigma}^*$ to be meaningful, the averages which define these effective quantities in (4.14) and (5.11) must be well defined and finite. For example, in order for the diagonal components D^*_{kk}, $k=1,\ldots,d$, of D^* to be well defined and finite, the vector field $\boldsymbol{\nabla}\chi_k$ must be Lebesgue measurable and square integrable on $\mathcal{T}\times\mathcal{V}$. Moreover, for the components A^*_{jk}, $j\neq k=1,\ldots,d$, of A^* to be well defined and finite, we must also have that the operator $\mathbf{S}$ is bounded in some sense so that $\mathbf{S}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k$ is Lebesgue integrable on $\mathcal{T}\times\mathcal{V}$. In other words, we must define the vector field $\boldsymbol{\nabla}\chi_j$ as a member of a suitable space of functions so that the components of the tensors D^* and $\boldsymbol{\sigma}^*$ are well defined and have finite values. In Section 6 we discuss these important details at length and prove the following theorem.

THEOREM 5.1. *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* (4.15)–(4.14) *and* (5.10)–(5.11), *respectively. Then there exists a function space* $\mathcal{F}$ *on which* $\boldsymbol{\sigma}=\varepsilon\mathsf{I}+\mathbf{S}$ *is a bounded linear operator for all* $0<\varepsilon<\infty$ *and, for* $\boldsymbol{\nabla}\chi_j\in\mathcal{F}$, D^*_{jk} *and* σ^*_{jk} *are well defined and finite. Moreover, these effective tensors are equivalent up to transposition,*

$$\boldsymbol{\sigma}^*=[\mathsf{D}^*]^T. \tag{5.12}$$

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* $\boldsymbol{\sigma}^*$.

Theorem 5.1 places the effective parameter problems for transport in composites and that for transport by advective diffusion on common mathematical footing, for both cases of time-independent and time-dependent velocity fields $\boldsymbol{u}$. The validity of Theorem 5.1 follows by adapting the Hilbert space formulation of the analytic continuation method to treat the effective transport properties of advective diffusion, which is the topic of Section 6. This Hilbert space formulation of the effective parameter problem also leads to integral representations for D^* and A^*, which is the topic of Section 7.

6. Hilbert space and resolvent representation. In this section we explore the mathematical properties of the skew-symmetric operator $\mathbf{S}$ introduced in equation (4.14) and construct a function space $\mathcal{F}$ such that for $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$ equation (5.12) holds and is well defined. We do so by providing an abstract Hilbert space formulation of the effective parameter problem for advective diffusion. We utilize this mathematical framework and equation (4.15) to obtain a resolvent representation of the vector field $\boldsymbol{\nabla}\chi_k$, involving an anti-symmetric operator $\mathbf{A}$ which is closely related to $\mathbf{S}$, where we use the terms skew-symmetric and anti-symmetric interchangeably. Using the results of this section, we derive in Section 7 integral representations for the symmetric D^* and anti-symmetric A^* parts of the effective diffusivity tensor D^*, involving a *spectral measure* associated with $\mathbf{A}$.

Consider the Hilbert spaces over the complex field $\mathbb{C}$ $L^2_d(\mathcal{T})=\otimes_{n=1}^d L^2(\mathcal{T})$ and $L^2_d(\mathcal{V})=\otimes_{n=1}^d L^2(\mathcal{V})$ of Lebesgue measurable, square integrable, vector-valued functions [32], where $\mathcal{T}\subset\mathbb{R}$ and $\mathcal{V}\subset\mathbb{R}^d$. Now consider the associated Hilbert spaces $\mathcal{H}_\mathcal{T}\subset L^2_d(\mathcal{T})$ and $\mathcal{H}_\mathcal{V}\subset L^2_d(\mathcal{V})$ of periodic vector-valued functions with temporal periodicity T on the interval $\mathcal{T}=(0,T)$ and spatial periodicities V_j, $j=1,\ldots,d$, on the d-dimensional region $\mathcal{V}=(0,V_1)\times\cdots\times(0,V_d)$, respectively, as well as their direct product $\mathcal{H}_{\mathcal{T}\mathcal{V}}$,

$$\mathcal{H}_{\mathcal{T}\mathcal{V}}=\mathcal{H}_\mathcal{T}\otimes\mathcal{H}_\mathcal{V},\quad \mathcal{H}_\mathcal{T}=\{\boldsymbol{\psi}\in L^2_d(\mathcal{T})\mid\boldsymbol{\psi}(0)=\boldsymbol{\psi}(T)\},\quad \mathcal{H}_\mathcal{V}=\{\boldsymbol{\psi}\in L^2_d(\mathcal{V})\mid\boldsymbol{\psi}(0)=\boldsymbol{\psi}(\boldsymbol{u})\}, \tag{6.1}$$

where we have defined $\boldsymbol{u}=(V_1,\ldots,V_d)$. Denote by $\langle\cdot,\cdot\rangle$ the sesquilinear inner-product associated with the Hilbert space $\mathcal{H}_{\mathcal{T}\mathcal{V}}$, which is defined by $\langle\boldsymbol{\psi},\boldsymbol{\varphi}\rangle=\langle\overline{\boldsymbol{\psi}}\cdot\boldsymbol{\varphi}\rangle$ with $\langle\boldsymbol{\psi},\boldsymbol{\varphi}\rangle=\overline{\langle\boldsymbol{\varphi},\boldsymbol{\psi}\rangle}$, where $\bar{a}$ denotes complex conjugation for $a\in\mathbb{C}$ and $(\overline{\boldsymbol{\psi}})_j=\overline{\psi_j}$, $j=1,\ldots,d$. By the Helmholtz theorem [54, 10], the Hilbert space $\mathcal{H}_\mathcal{V}$ in (4.10) can be decomposed into mutually orthogonal subspaces of curl-free $\mathcal{H}_W$, divergence-free $\mathcal{H}_\bullet$, and constant $\mathcal{H}_0$ vector fields, with associated orthogonal projectors Γ_W, $\Gamma_\bullet$, and Γ_0, respectively, [27, 63]

$$\begin{gathered}\mathcal{H}_\mathcal{V}=\mathcal{H}_W\oplus\mathcal{H}_\bullet\oplus\mathcal{H}_0,\qquad \mathsf{I}=\Gamma_W+\Gamma_\bullet+\Gamma_0,\\ \Gamma_W=\boldsymbol{\nabla}(\Delta^{-1})\boldsymbol{\nabla}\cdot,\quad \Gamma_\bullet=-\boldsymbol{\nabla}W(\boldsymbol{\Delta}^{-1})\boldsymbol{\nabla}W,\quad \Gamma_0=\langle\cdot\rangle,\\ \mathcal{H}_W=\{\boldsymbol{\psi}\mid\boldsymbol{\nabla}W\boldsymbol{\psi}=0\text{ weakly}\},\quad \mathcal{H}_\bullet=\{\boldsymbol{\psi}\mid\boldsymbol{\nabla}\cdot\boldsymbol{\psi}=0\text{ weakly}\},\quad \mathcal{H}_0=\{\boldsymbol{\psi}\mid\boldsymbol{\psi}=\langle\boldsymbol{\psi}\rangle\}.\end{gathered} \tag{6.2}$$

We are primarily concerned with fluid velocity fields $\boldsymbol{u}$ such that $0<\mathsf{D}^*_{kk}<\infty$ for all $0<\varepsilon<\infty$. Consequently, in view of equation (4.14), we require that the (weakly) curl-free vector field $\boldsymbol{\nabla}\chi_k$ satisfies $\boldsymbol{\nabla}\chi_k\in\mathcal{H}_\mathcal{T}\otimes\mathcal{H}_W\subset\mathcal{H}_{\mathcal{T}\mathcal{V}}$, so that it is bounded in the norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{T}\mathcal{V}}$-inner-product [32], $\|\boldsymbol{\nabla}\chi_k\|<\infty$. Defining the (weakly) divergence-free vector field $\boldsymbol{J}_k=\boldsymbol{\sigma}\boldsymbol{e}_k$ in (5.10) as a member of a subset of $\mathcal{H}_{\mathcal{T}\mathcal{V}}$ is technically difficult, due to the *unboundedness* of the linear operator $\boldsymbol{\sigma}=\mathsf{D}-(\boldsymbol{\Delta}^{-1})\mathbf{T}$ on this space. We now explore the properties of this operator in more detail.

Since $\mathcal{V}$ is a bounded domain, (Δ^{-1}) is a compact operator [83] on the Hilbert space $L^2(\mathcal{V})$. Hence $(\boldsymbol{\Delta}^{-1})$ is a compact operator on the Hilbert space $\mathcal{H}_\mathcal{V}$, and is consequently bounded in the operator norm $\|\cdot\|$ induced by the $\mathcal{H}_{\mathcal{T}\mathcal{V}}$-inner-product [77, 85, 83], when considered as an operator on $\mathcal{H}_{\mathcal{T}\mathcal{V}}$. We have already assumed for the convergence $\phi^\delta\to\bar{\phi}$, as $\delta\to0$, that the flow matrix $\mathsf{H}(t,\boldsymbol{x})$ is periodic on $\mathcal{T}\times\mathcal{V}$. We will also assume that it is (component-wise) mean-zero and bounded in operator norm, and that its component-wise time derivative $\mathbf{T}\mathsf{H}$ is also bounded on $\mathcal{H}_{\mathcal{T}\mathcal{V}}$

$$\langle\mathsf{H}\rangle=0,\quad\|\mathsf{H}\|<\infty,\quad\|\mathbf{T}\mathsf{H}\|<\infty. \tag{6.3}$$

This implies that $\mathsf{D} = \varepsilon\mathsf{I} + \mathsf{H}$ is also bounded for all $0 < \varepsilon < \infty$. Consequently, in the case of a time-independent velocity field $\boldsymbol{u}$, where $\boldsymbol{\sigma} = \mathsf{D}$, the linear operator $\boldsymbol{\sigma}$ is bounded. This and $\|\boldsymbol{\nabla}\chi_k\| < \infty$ implies that $\boldsymbol{J}_k \in \mathcal{H}_\bullet$. Therefore, in the case of a time-dependent velocity field, under the assumptions of (6.3), the unboundedness of $\boldsymbol{\sigma} = \mathsf{D} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ on $\mathcal{H}_{\mathcal{T}\mathcal{V}}$ is due to the unboundedness of $\mathbf{T}$ on $\mathcal{H}_\mathcal{T}$.

Proof of Theorem 5.1. 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 (5.10) 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 (6.3). 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 $\boldsymbol{\nabla}\chi_k \in \mathcal{H}_\mathcal{T} \otimes \mathcal{H}_W$. Therefore, this and equation (4.15) suggest that we consider the curl-free, mean-zero vector field $\boldsymbol{\nabla}\chi_k$ as a member of the function space $\mathcal{F} \subset \mathcal{F}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}$,

$$\mathcal{F} = \{\boldsymbol{\psi} \in \mathcal{F}_\mathcal{T} \otimes \mathcal{H}_W \mid \langle \boldsymbol{\psi} \rangle = 0\}, \tag{6.4}$$

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 $\mathcal{H}_\mathcal{T} \otimes \mathcal{H}_W$. 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 (6.4), so that $\boldsymbol{\psi} \in \mathcal{F}$ implies $\boldsymbol{\psi} \in \mathcal{H}_W$ 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 $\mathcal{H}_W$ and $\mathcal{H}_\bullet$ in equation (4.11), $\boldsymbol{\nabla}\chi_k \in \mathcal{F}$, $\boldsymbol{J}_k \in \mathcal{H}_\mathcal{T} \otimes \mathcal{H}_\bullet$, and Fubini's theorem [32] 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 (5.10) and (5.11) 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,

$$\sigma^*_{jk} = \varepsilon\langle \boldsymbol{e}_j \cdot \boldsymbol{e}_k \rangle + \langle \mathbf{S}\boldsymbol{e}_j \cdot \boldsymbol{e}_k \rangle. \tag{6.5}$$

The property $\langle \boldsymbol{\nabla}\chi_k \rangle = 0$ in (4.15), and equation (4.14) together imply that

$$\varepsilon\langle \boldsymbol{e}_j \cdot \boldsymbol{e}_k \rangle = \varepsilon[\langle \boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k \rangle + \langle \boldsymbol{\nabla}\chi_j \cdot \boldsymbol{e}_k \rangle + \langle \boldsymbol{e}_j \cdot \boldsymbol{\nabla}\chi_k \rangle + \langle \boldsymbol{e}_j \cdot \boldsymbol{e}_k \rangle] = \varepsilon(\langle \boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k \rangle + \delta_{jk}) = \mathsf{S}^*_{jk}. \tag{6.6}$$

From the definition of $\mathbf{S} = \mathsf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ in equation (4.14) 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 (6.3) the matrix H is (component-wise) mean-zero. Also, by the definition $\boldsymbol{u} = \boldsymbol{\nabla} \cdot \mathsf{H}$ in (4.13) 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 (4.14), (A.12), and (4.17), we have

$$\begin{aligned}
\langle \mathbf{S}\boldsymbol{e}_j \cdot \boldsymbol{e}_k \rangle &= \langle \mathbf{S}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k \rangle + \langle \mathbf{S}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{e}_k \rangle + \langle \mathbf{S}\boldsymbol{e}_j \cdot \boldsymbol{\nabla}\chi_k \rangle + \langle \mathbf{S}\boldsymbol{e}_j \cdot \boldsymbol{e}_k \rangle \\
&= \mathsf{A}^*_{jk} - \langle \boldsymbol{\nabla}\chi_j \cdot \mathsf{H}\boldsymbol{e}_k \rangle + \langle \mathsf{H}\boldsymbol{e}_j \cdot \boldsymbol{\nabla}\chi_k \rangle \\
&= \mathsf{A}^*_{jk} + \langle \chi_j u_k \rangle - \langle u_j \chi_k \rangle \\
&= \mathsf{A}^*_{jk} + [\mathsf{A}^*_{kj} + \mathsf{S}^*_{kj} - \varepsilon\delta_{kj}] - [\mathsf{A}^*_{jk} + \mathsf{S}^*_{jk} - \varepsilon\delta_{jk}] \\
&= -\mathsf{A}^*_{jk}.
\end{aligned} \tag{6.7}$$

In summary, from equations (6.5)–(6.7) and the symmetries $\mathsf{S}^*_{jk} = \mathsf{S}^*_{kj}$ and $\mathsf{A}^*_{jk} = -\mathsf{A}^*_{kj}$ we have that

$$\sigma^*_{jk} = \mathsf{S}^*_{jk} - \mathsf{A}^*_{jk} = \mathsf{S}^*_{kj} + \mathsf{A}^*_{kj} = \mathsf{D}^*_{kj}\,, \tag{6.8}$$

which is equivalent to equation (5.12). This concludes our proof of Theorem 5.1 $\Box$.

We conclude this section with a derivation of the following resolvent formula for $\boldsymbol{\nabla}\chi_k$, involving the orthogonal projection operator $\Gamma_W = \boldsymbol{\nabla}(\Delta^{-1})\boldsymbol{\nabla}\cdot$ onto curl-free fields in (4.11),

$$\boldsymbol{\nabla}\chi_j = (\varepsilon\mathsf{I} + \mathbf{A})^{-1}\boldsymbol{g}_j = (\varepsilon\mathsf{I} + \imath\mathbf{M})^{-1}\boldsymbol{g}_j, \quad \mathbf{A} = \Gamma\mathbf{S}\Gamma, \quad \mathbf{M} = -\imath\mathbf{A}, \quad \boldsymbol{g}_j = -\Gamma\mathsf{H}\boldsymbol{e}_j, \tag{6.9}$$

where $\imath=\sqrt{-1}$ and we have defined $\Gamma=\Gamma_W$ for notational simplicity. Equation (6.9) follows from applying the integro-differential operator $\boldsymbol{\nabla}(\Delta^{-1})$ to $\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\boldsymbol{e}_j=0$ in equation (5.10), with $\boldsymbol{e}_j=\boldsymbol{\nabla}\chi_j+\boldsymbol{e}_j$ and $\boldsymbol{\sigma}=\varepsilon\mathsf{I}+\mathbf{S}$, yielding

$$\Gamma(\varepsilon\mathsf{I}+\mathbf{S})\boldsymbol{\nabla}\chi_j=-\Gamma\mathsf{H}\boldsymbol{e}_j, \tag{6.10}$$

since $\Gamma\boldsymbol{e}_j=0$ and $\mathbf{S}\boldsymbol{e}_j=\mathsf{H}\boldsymbol{e}_j$. The equivalence of equations (6.9) and (6.10) can be seen by noting that $\boldsymbol{\nabla}\chi_j\in\mathcal{F}$ implies $\Gamma\boldsymbol{\nabla}\chi_j=\boldsymbol{\nabla}\chi_j$. We stress that the property $\Gamma\boldsymbol{\nabla}\chi_j=\boldsymbol{\nabla}\chi_j$ implies that $\mathbf{A}\boldsymbol{\nabla}\chi_j=\Gamma\mathbf{S}\Gamma\boldsymbol{\nabla}\chi_j=\Gamma\mathbf{S}\boldsymbol{\nabla}\chi_j=(\Gamma\mathsf{H}-\boldsymbol{\Delta}^{-1}\mathbf{T})\boldsymbol{\nabla}\chi_j$.

It is worth mentioning that taking the $\ell^2(\mathbb{C}^N)$ inner-product of both sides of equation (6.10) with $\boldsymbol{\nabla}\chi_k$, averaging, using the properties $\Gamma\boldsymbol{\nabla}\chi_j=\boldsymbol{\nabla}\chi_j$ and $\langle\Gamma\boldsymbol{\psi}\cdot\boldsymbol{\varphi}\rangle=\langle\boldsymbol{\psi}\cdot\Gamma\boldsymbol{\varphi}\rangle$ for $\boldsymbol{\psi},\boldsymbol{\varphi}\in\mathcal{H}_{\mathcal{V}}$, and integrating by parts, yields equation (4.17). Moreover, the condition $\langle\boldsymbol{J}_j\cdot\boldsymbol{\nabla}\chi_k\rangle=0$ is also equivalent to equation (4.17).

In Section A.1 we show that $\mathbf{A}$ in (6.9) acts as an anti-symmetric linear operator on the Hilbert space $\mathcal{H}_{\mathcal{T}\mathcal{V}}$, $\langle\mathbf{A}\boldsymbol{\psi}\cdot\boldsymbol{\varphi}\rangle=\langle\boldsymbol{\psi}\cdot\mathbf{A}^*\boldsymbol{\varphi}\rangle=-\langle\boldsymbol{\psi}\cdot\mathbf{A}\boldsymbol{\varphi}\rangle$. Therefore, $\mathbf{A}$ commutes with its (Hilbert space) adjoint $\mathbf{A}^*=-\mathbf{A}$ (not to be confused with an effective tensor) and is therefore an example of a *normal* operator [85]. Consequently, due to the sesquilinearity of the $\mathcal{H}_{\mathcal{T}\mathcal{V}}$-inner-product, $\mathbf{M}=-\imath\mathbf{A}$ acts as a *symmetric* operator, $\mathbf{M}^*=\mathbf{M}$ [77, 85]. Moreover, on the function space $\mathcal{F}$, $\mathbf{A}$ is a *maximal* normal operator and $\mathbf{M}$ is *self-adjoint* [85]. In Section 7 we examine these properties of $\mathbf{A}$ and $\mathbf{M}$ in more detail and demonstrate how equation (6.9) and the spectral theory of such operators lead to integral representations for the symmetric D^* and anti-symmetric A^* parts of D^*.

7. Integral representations of the effective diffusivity. In this section, we employ the Hilbert space formulation of the effective parameter problem discussed in Section 6 above, to provide integral representations for the symmetric D^* and anti-symmetric A^* parts of the effective diffusivity tensor D^*, for steady and dynamic flows. In the general (infinite dimensional) setting, these integral representations involve a *spectral measure* $\mathrm{d}\boldsymbol{\mu}$ associated with the (maximal) normal operator $\mathbf{A}=\Gamma\mathbf{S}\Gamma$ on $\mathcal{F}$, or equivalently the self-adjoint operator $\mathbf{M}=-\imath\mathbf{A}$, and follow from the spectral theorem for such linear operators [77, 85] and the resolvent formula for $\boldsymbol{\nabla}\chi_k$ given in equation (6.9). The derivation of these integral representations for D^* and A^* is the topic of Section 7.1. In Section 7.2 we discuss an important alternate formulation of the effective parameter problem, where the spatial Hilbert space $\mathcal{H}_W$ is replaced by a Sobolev space $\mathscr{H}^1_{\mathcal{V}}$. In Section 7.3 we demonstrate that the two approaches are equivalent, and are in isometric correspondence. The spectral measures underlying these integral representations have discrete and continuous components. In Section A.4 we review this theory and provide an explicit derivation of the discrete component of these integrals, by eigenfunction expansion. In Sections **??** and **??** we discuss the mathematical framework of these two approaches in the finite dimensional setting, where the underlying operators are given by matrices. This spectral analysis illuminates a great deal of structure regarding the spectral measure $\mathrm{d}\boldsymbol{\mu}$ in this matrix setting. This structure is utilized in Section 10 to formulate an efficient and stable numerical algorithm for the explicit computation of D^* and A^* for model velocity fields $\boldsymbol{u}$, by the direct computation of $\mathrm{d}\boldsymbol{\mu}$ in terms of the eigenvalues and eigenvectors of $\mathbf{A}$.

7.1. General infinite dimensional setting - curl free. In the general Hilbert space setting, there are significant differences in the theory between the case of steady flows, where $\mathbf{S}=\mathsf{H}$ is *bounded* on the Hilbert space $\mathcal{H}_{\mathcal{V}}$, and the case of dynamic flows, where $\mathbf{S}=\mathsf{H}-(\boldsymbol{\Delta}^{-1})\mathbf{T}$ is *unbounded* on the Hilbert space $\mathcal{H}_{\mathcal{T}\mathcal{V}}$, as discussed in Section 6. It is therefore natural to start our discussion with a more detailed look into this distinction, in the present context. Since Γ is an orthogonal projector from $\mathcal{H}_{\mathcal{V}}$ to $\mathcal{H}_W$, it is bounded by unity in operator norm $\|\Gamma\|\le 1$ on $\mathcal{H}_{\mathcal{V}}$ and $\|\Gamma\|=1$ on $\mathcal{H}_W$ [77, 85]. Therefore by (6.3), in the case of steady flows, the operator $\mathbf{A}=\Gamma\mathsf{H}\Gamma$ is bounded on the Hilbert space $\mathcal{H}_{\mathcal{V}}$, with $\|\mathbf{A}\|\le\|\mathsf{H}\|<\infty$. Let's first focus on this time-independent case. Since $\mathbf{M}=-\imath\mathbf{A}$ we have $\|\mathbf{M}\|=\|\mathbf{A}\|$, so the domains of these two operators are identical, $D(\mathbf{M})=D(\mathbf{A})$. For simplicity we focus on the operator $\mathbf{M}$ now, re-introducing the operator $\mathbf{A}$ later. The (Hilbert space) adjoint $\mathbf{M}^*$ of $\mathbf{M}$ is defined by $\langle\mathbf{M}\psi,\varphi\rangle=\langle\psi,\mathbf{M}^*\varphi\rangle$, and is also a bounded operator on $\mathcal{H}_{\mathcal{V}}$ with $\|\mathbf{M}^*\|=\|\mathbf{M}\|$ [77]. Consequently, they have identical domains,

$$D(\mathbf{M})=D(\mathbf{M}^*), \tag{7.1}$$

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

$$\langle\mathbf{M}\boldsymbol{\psi}\cdot\boldsymbol{\varphi}\rangle=\langle\boldsymbol{\psi}\cdot\mathbf{M}\boldsymbol{\varphi}\rangle,\ \text{ for all }\ \boldsymbol{\psi},\boldsymbol{\varphi}\in D(\mathbf{M}). \tag{7.2}$$

By definition [77, 85], the two properties (3.1) and (3.2) together imply that the operator $\mathbf{M}$ is *self-adjoint*, i.e. $\mathbf{M} \equiv \mathbf{M}^*$ on $D(\mathbf{M})$.

Conversely, the Hellinger–Toeplitz theorem [77] states, if the operator $\mathbf{M}$ satisfies equation (3.2) for *every* $\boldsymbol{\psi}, \boldsymbol{\varphi} \in \mathcal{H}_\mathcal{V}$, then $\mathbf{M}$ is bounded on $\mathcal{H}_\mathcal{V}$. This suggests that, in the time-dependent case when $\mathbf{M}$ is unbounded on the Hilbert space $\mathcal{H}_{\mathcal{T}\mathcal{V}}$, it is defined as a self-adjoint operator only on a proper subset of $\mathcal{H}_{\mathcal{T}\mathcal{V}}$. However, as discussed in Section 6, the domain $D(\mathbf{M})$ can be defined as a *dense* subset of $\mathcal{H}_{\mathcal{T}\mathcal{V}}$ such that $\mathbf{M}$ is bounded. Moreover, on this domain, $\mathbf{M}$ can be extended to a *closed* symmetric operator [77, 85]. Although even in this case, in general [77], the domain $D(\mathbf{M}^*)$ of the associated adjoint $\mathbf{M}^*$ does not coincide with $D(\mathbf{M})$, and in such circumstances $\mathbf{M}$ is *not* self-adjoint on $D(\mathbf{M})$. Only for self-adjoint (or maximal normal) operators does the spectral theorem hold [77], which provides the existence of the promised integral representation for D^*, involving a spectral measure associated with $\mathbf{M}$. It is therefore necessary that we find a domain $D(\mathbf{M})$ on which $\mathbf{M}$ is self-adjoint.

As Γ is bounded on $\mathcal{H}_\mathcal{V}$ and $\mathbf{M} = -\imath\Gamma\mathbf{S}\Gamma$, our discussion in Section 6 indicates that the unboundedness of $\mathbf{M}$ on $\mathcal{H}_{\mathcal{T}\mathcal{V}}$ is due to the unboundedness of the underlying operator $\mathbf{T}$ on the Hilbert space $\mathcal{H}_\mathcal{T}$. It is therefore necessary that we find a domain $D(\mathbf{T})$ for which $\imath\mathbf{T}$ is a self-adjoint operator. Toward this goal, and to illustrate these ideas, we consider the operator $\imath\partial_t$ with the three different domains $\mathscr{A}_\mathcal{T}$, $\tilde{\mathscr{A}}_\mathcal{T}$, and $\hat{\mathscr{A}}_\mathcal{T}$ defined in equations (3.10) and (3.11), which are everywhere dense in $L^2(\mathcal{T})$ [85]. 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 adjoint $\hat{B}^* \equiv B$, and the operator $\tilde{B}$ is a *self-adjoint* extension of $\hat{B}$ [85]. 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 $\tilde{\mathscr{A}}_\mathcal{T}$.

Since the operator $\tilde{B} = \imath\partial_t$ with domain $\tilde{\mathscr{A}}_\mathcal{T}$ is self-adjoint, it follows that the operator $\imath\mathbf{T} = \imath\partial_t\mathsf{I}$ with domain $D(\mathbf{T}) = \mathcal{F}_\mathcal{T} = \otimes_{n=1}^d \tilde{\mathscr{A}}_\mathcal{T}$ is self-adjoint. This is seen as follows. By noting that $\imath\mathbf{T}\boldsymbol{\psi} = (\tilde{B}\psi_1, \ldots, \tilde{B}\psi_d)$ and, for all $\boldsymbol{\psi}, \boldsymbol{\varphi} \in \mathcal{F}_\mathcal{T}$ with components $\psi_j, \varphi_j \in \tilde{\mathscr{A}}_\mathcal{T}$, $j = 1, \ldots, d$, the self-adjointness of $\tilde{B}$ implies that $\mathbf{T}$ is symmetric, $\mathbf{T} = \mathbf{T}^*$, on $\mathcal{F}_\mathcal{T}$,

$$\langle \mathbf{T}\boldsymbol{\psi} \cdot \boldsymbol{\varphi} \rangle = \sum_j \langle \tilde{B}\psi_j, \varphi_j \rangle_2 = \sum_j \langle \psi_j, \tilde{B}\varphi_j \rangle_2 = \langle \boldsymbol{\psi} \cdot \mathbf{T}\boldsymbol{\varphi} \rangle, \tag{7.3}$$

where $\langle \cdot, \cdot \rangle_2$ denotes the $L^2(\mathcal{T})$-inner-product. Moreover, since we have $D(\tilde{B}) = D(\tilde{B}^*) = \tilde{\mathscr{A}}_\mathcal{T}$, we also have $D(\mathbf{T}) = D(\mathbf{T}^*) = \mathcal{F}_\mathcal{T}$, i.e. $\mathbf{T} \equiv \mathbf{T}^*$ on $\mathcal{F}_\mathcal{T}$. Consequently, $\mathbf{T}$ is a bounded self-adjoint linear operator on the function space $\mathcal{F}_\mathcal{T}$.

We now summarize what we have discussed so far, and discuss the implications thereof. We have discussed that the operators $(\boldsymbol{\Delta}^{-1})$ and Γ are bounded on the Hilbert space $\mathcal{H}_\mathcal{V}$. In Section A.1 we show that they are also symmetric, hence self-adjoint on $\mathcal{H}_\mathcal{V}$. Due to the sesquilinearity of the $\mathcal{H}_{\mathcal{T}\mathcal{V}}$-inner-product, and equations (6.3) and (4.13) with $\mathsf{H}^* = \mathsf{H}^T$, the operator $\imath\mathsf{H}$ is bounded and symmetric, hence self-adjoint on the Hilbert space $\mathcal{H}_{\mathcal{T}\mathcal{V}}$. Consequently, the operator $\imath\Gamma\mathsf{H}\Gamma$ is also self-adjoint on $\mathcal{H}_{\mathcal{T}\mathcal{V}}$. The differential and integral operators $\imath\mathbf{T}$ and $(\boldsymbol{\Delta}^{-1})$ are bounded on the function space $\mathcal{F}_\mathcal{T}$ and Hilbert space $\mathcal{H}_\mathcal{V}$, respectively, and they are consequently commutable operations on the function space $\mathcal{F}_\mathcal{T} W \mathcal{H}_\mathcal{V}$ [32]. Moreover, as $\imath\mathbf{T}$ and $(\boldsymbol{\Delta}^{-1})$ are self-adjoint on $\mathcal{F}_\mathcal{T}$ and $\mathcal{H}_\mathcal{V}$, respectively, the operator $\imath(\boldsymbol{\Delta}^{-1})\mathbf{T}$, hence $\imath\Gamma[(\boldsymbol{\Delta}^{-1})\mathbf{T}]\Gamma$ is self-adjoint on $\mathcal{F}_\mathcal{T} W \mathcal{H}_\mathcal{V}$. It is now clear that the operator $\mathbf{M} = \imath\Gamma\mathbf{S}\Gamma$, with $\mathbf{S} = \mathsf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$, is self-adjoint on $\mathcal{F}_\mathcal{T} W \mathcal{H}_\mathcal{V}$. Finally, since $\mathbf{M} = -\imath\mathbf{A}$ is self-adjoint on $\mathcal{F}_\mathcal{T} W \mathcal{H}_\mathcal{V}$ and an operator is self-adjoint if and only if it is a maximal normal operator [85], we have that $\mathbf{A}$ is a maximal normal operator on $\mathcal{F}_\mathcal{T} W \mathcal{H}_\mathcal{V}$. In view of the resolvent formulas for $\boldsymbol{\nabla}\chi_j \in \mathcal{F}$ in (6.9) involving $\mathbf{M}$ and $\mathbf{A}$, we will henceforth take the domain of these operators to be $D(\mathbf{A}) = D(\mathbf{M}) = \mathcal{F}$ in (6.4), which is a *closed* subset of $\mathcal{F}_\mathcal{T} W \mathcal{H}_\mathcal{V}$.

In terms of a general, maximal normal operator $\mathbf{N}$ on $\mathcal{F}$ satisfying $\mathbf{N}\mathbf{N}^* = \mathbf{N}^*\mathbf{N}$, the spectral theorem states that $\mathbf{N}$ can be decomposed as $\mathbf{N} = \mathsf{H}_1 + \imath\mathsf{H}_2$, where H_1 and H_2 are self-adjoint and commute on $\mathcal{F}$ [85]. Moreover, there is a one-to-one correspondence between H_n, $n = 1, 2$, and a family $\{\mathbf{Q}_n(\lambda)\}$, $-\infty < \lambda < \infty$, of self-adjoint projection operators - the resolution of the identity - with domain $\mathcal{F}$ which satisfies $\lim_{\lambda\to-\infty} \mathbf{Q}_n(\lambda) = 0$, $\lim_{\lambda\to+\infty} \mathbf{Q}_n(\lambda) = \mathsf{I}$, and the $\mathbf{Q}_n(\lambda)$, $n = 1, 2$, commute [77, 85]. Consequently, there is a one-to-one correspondence between $\mathbf{N}$ and a family $\{\mathbf{Q}(z)\}$, $\mathbf{Q}(z) = \mathbf{Q}_1(\mathrm{Re}(z))\mathbf{Q}_2(\mathrm{Im}(z))$, $z = \lambda_1 + \imath\lambda_2$, $-\infty < \lambda_1, \lambda_2 < \infty$, of self-adjoint projection operators - the *complex* resolution of the identity - which satisfies $\mathbf{Q}(z) \to 0$ when $\mathrm{Re}(z) \to -\infty$ and when $\mathrm{Im}(z) \to -\infty$, and $\mathbf{Q}(z) \to \mathsf{I}$ when $\mathrm{Re}(z) \to +\infty$ and when $\mathrm{Im}(z) \to +\infty$ [85].

The spectral theorem also provides an operational calculus in Hilbert space which yields integral representations associated with $\mathbf{Q}(z)$-measurable functions of $\mathbf{N}$ [85]. The details are as follows. Let $\boldsymbol{\psi}, \boldsymbol{\varphi} \in \mathcal{F}$

and consider the *complex-valued* function $\mu_{\psi\varphi}(z) = \langle \mathbf{Q}(z)\boldsymbol{\psi} \cdot \boldsymbol{\varphi}\rangle$, $\boldsymbol{\psi} \neq \boldsymbol{\varphi}$. By the sesquilinearity of the inner-product and the self-adjointness of the projection operator $\mathbf{Q}(z)$ we have $\mu_{\varphi\psi}(z) = \overline{\mu}_{\psi\varphi}(z)$, where $\overline{\mu}_{\psi\varphi}$ denotes the complex conjugate of $\mu_{\psi\varphi}$. Moreover, the function $\mu_{\psi\psi}$ is real-valued and positive $\mu_{\psi\psi}(z) = \langle \mathbf{Q}(z)\boldsymbol{\psi} \cdot \boldsymbol{\psi}\rangle = \langle \mathbf{Q}(z)\boldsymbol{\psi} \cdot \mathbf{Q}(z)\boldsymbol{\psi}\rangle = \|\mathbf{Q}(z)\boldsymbol{\psi}\|^2$. We associate with these functions of *bounded variation* Radon–Stieltjes measures $\mathrm{d}\mu_{\psi\varphi}(z)$ and $\mathrm{d}\mu_{\psi\psi}(z)$ [85]

$$\mathrm{d}\mu_{\psi\varphi}(z) = \mathrm{d}\langle \mathbf{Q}(z)\boldsymbol{\psi} \cdot \boldsymbol{\varphi}\rangle, \quad \boldsymbol{\psi} \neq \boldsymbol{\varphi}, \qquad \mathrm{d}\mu_{\psi\psi}(z) = \mathrm{d}\|\mathbf{Q}(z)\boldsymbol{\psi}\|^2. \tag{7.4}$$

Let $F(z)$ be an arbitrary complex-valued function and denote by $\mathscr{D}(F)$ the set of all $\boldsymbol{\psi} \in \mathcal{F}$ such that $F \in L^2(\mu_{\psi\psi})$, i.e. $F(z)$ is square integrable with respect to the measure $\mathrm{d}\mu_{\psi\psi}$. Then $\mathscr{D}(F)$ is a linear manifold and there exists a linear transformation $F(\mathbf{N})$ with domain $\mathscr{D}(F)$ defined in terms of the Radon–Stieltjes integrals [85]

$$\langle F(\mathbf{N})\boldsymbol{\psi} \cdot \boldsymbol{\varphi}\rangle = \int_I \overline{F}(z)\,\mathrm{d}\mu_{\psi\varphi}(z), \qquad \forall\,\boldsymbol{\psi} \in \mathscr{D}(F),\ \boldsymbol{\varphi} \in \mathcal{F} \tag{7.5}$$
$$\langle F(\mathbf{N})\boldsymbol{\psi} \cdot G(\mathbf{N})\boldsymbol{\varphi}\rangle = \int_I \overline{F}(z)G(z)\,\mathrm{d}\mu_{\psi\varphi}(z), \quad \forall\,\boldsymbol{\psi} \in \mathscr{D}(F),\ \boldsymbol{\varphi} \in \mathscr{D}(G),$$

where the operator $G(\mathbf{N})$ and function space $\mathscr{D}(G)$ are defined analogously to that for F. An integral representation for the functional $\|F(\mathbf{N})\boldsymbol{\psi}\|^2$ follows from the second formula in (3.6) with $G = F$ and $\boldsymbol{\psi} = \boldsymbol{\varphi}$, and involves the measure $\mathrm{d}\mu_{\psi\psi}$ in (3.5) [85]. The domain of integration I in (3.6) is the *spectrum* $\Sigma(\mathbf{N})$ of the operator $\mathbf{N}$, $I \equiv \Sigma(\mathbf{N})$. Since $\mathbf{N}$ is a normal operator, its norm $\|\mathbf{N}\|$ coincides with the spectral radius $\|\mathbf{N}\| = \sup\{|z| : z \in \Sigma(\mathbf{N})$, so that in general $I \subseteq (-\infty,\infty)W(-\imath\infty,\imath\infty)$ [77, 85].

The spectral theorem of equation (3.6) for the maximal normal operator $\mathbf{N}$ on $\mathcal{F}$ generalizes that for self-adjoint and maximal anti-symmetric operators, with purely real and imaginary spectrum, respectively. More specifically, the case $F(z) = z = \lambda_1 + \imath\lambda_2$ corresponds to $F(\mathbf{N}) = \mathsf{H}_1 + \imath\mathsf{H}_2$ with $I \subseteq (-\infty,\infty)W(-\imath\infty,\imath\infty)$ and $\mathbf{Q}(z) = \mathbf{Q}_1(\mathrm{Re}(z))\mathbf{Q}_2(\mathrm{Im}(z))$, the case $F(z) = \mathrm{Re}(z)$ corresponds to the self-adjoint operator $F(\mathbf{N}) = \mathsf{H}_1$ with $I \subseteq (-\infty,\infty)$ and $\mathbf{Q}(z) = \mathbf{Q}_1(\mathrm{Re}(z))$, and the case $F(z) = \imath\,\mathrm{Im}(z)$ corresponds to the maximal anti-symmetric operator $F(\mathbf{N}) = \imath\mathsf{H}_2$ with $I \subseteq (-\imath\infty,\imath\infty)$ and $\mathbf{Q}(z) = \mathbf{Q}_2(\mathrm{Im}(z))$ [85]. We now apply the spectral theorem to equations (4.14) and (6.9) to provide Radon–Stieltjes integral representations for the symmetric D^* and anti-symmetric A^* parts of the effective diffusivity tensor D^*, for both cases of time-independent and time-dependent velocity fields $\boldsymbol{u}$. These representations are summarized by the following theorem.

Theorem 7.1. *Let $z = \imath\lambda$, $\boldsymbol{g}_j = -\Gamma\mathsf{H}\boldsymbol{e}_j$ be defined as in* (6.9)*, and $\mathbf{Q}(z) = \mathbf{Q}_2(\mathrm{Im}(z)) = \mathbf{Q}_2(\lambda)$ be the complex resolution of the identity associated with the maximal anti-symmetric operator $\mathbf{A}$ defined in* (6.9)*, with domain $\mathcal{F}$ defined in* (6.4)*. Define the matrix-valued function $\boldsymbol{\mu}(\lambda)$ with complex-valued off-diagonal components $\mu_{jk}(\lambda) = \langle \mathbf{Q}_2(\lambda)\boldsymbol{g}_j \cdot \boldsymbol{g}_k\rangle$ for $j \neq k = 1,\ldots,d$, with $\mu_{kj} = \overline{\mu}_{jk}$, and positive diagonal components $\mu_{kk}(\lambda) = \|\mathbf{Q}_2(\lambda)\boldsymbol{g}_k\|^2$. Moreover, consider the real-valued functions*

$$\mathrm{Re}\,\mu_{jk}(\lambda) = \frac{1}{2}\left(\mu_{jk}(\lambda) + \overline{\mu}_{jk}(\lambda)\right), \quad \mathrm{Im}\,\mu_{jk}(\lambda) = \frac{1}{2\imath}\left(\mu_{jk}(\lambda) - \overline{\mu}_{jk}(\lambda)\right). \tag{7.6}$$

Corresponding to each of these functions of bounded variation, consider the associated Radon–Stieltjes measures $\mathrm{d}\mu_{jk}(\lambda)$, $\mathrm{d}\mu_{kk}(\lambda)$, $\mathrm{dRe}\,\mu_{jk}(\lambda)$, and $\mathrm{dIm}\,\mu_{jk}(\lambda)$. Then, for all $0 < \varepsilon < \infty$, there exist Radon–Stieltjes integral representations for the components S^*_{jk} and A^*_{jk}, $j,k = 1,\ldots,d$, of the effective tensors D^* and A^* defined in equation (4.14)*, given by*

$$\mathsf{S}^*_{jk} = \varepsilon\left(\delta_{jk} + \int_{-\infty}^{\infty} \frac{\mathrm{dRe}\,\mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2}\right), \qquad \mathsf{A}^*_{jk} = \int_{-\infty}^{\infty} \frac{\lambda\,\mathrm{dIm}\,\mu_{jk}(\lambda)}{\varepsilon^2 + \lambda^2}\,. \tag{7.7}$$

Here, the domain of integration I is determined by the spectrum $\Sigma(\mathbf{A})$ of the operator $\mathbf{A}$, where $I \subseteq [-\|\mathbf{A}\|, \|\mathbf{A}\|]$ and $\|\mathbf{A}\| \leq \|\mathsf{H}\| < \infty$ in the case of a time-independent velocity field $\boldsymbol{u}$ [77].

A key feature of the integral representations for D^* and A^* in (7.7) is that parameter information in ε is *separated* from the geometry and dynamics of the velocity field $\boldsymbol{u}$, which are encapsulated in the underlying spectral measure $\mathrm{d}\boldsymbol{\mu}$. In Section A.4 we will discuss in more detail the properties of the spectrum $\Sigma(\mathbf{A})$ of the operator $\mathbf{A}$. Moreover, we show how these properties of Σ lead to useful decompositions of the measure $\mathrm{d}\boldsymbol{\mu}$. These measure decompositions are employed in Section 8 to calculate S^*_{jk} and A^*_{jk} for a large class of velocity fields $\boldsymbol{u}$. Furthermore, in Section **??** these important properties of the integrals in (7.7) lead to asymptotic behavior of D^* and A^* in the advection and diffusion dominated regimes, where the molecular diffusivity tends to zero, $\varepsilon \to 0$, and infinity, $\varepsilon \to \infty$, respectively.

Proof of Theorem 7.1. We first note that from $\boldsymbol{\nabla}\chi_k \in \mathcal{F}$ we have $\boldsymbol{\nabla}\chi_k = \Gamma\boldsymbol{\nabla}\chi_k$, so that A^*_{jk} in equation (4.14) can re-expressed as $\mathsf{A}^*_{jk} = \langle \mathbf{S}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle \Gamma\mathbf{S}\Gamma\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle \mathbf{A}\boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle$, where we have used that Γ is self-adjoint on $\mathcal{F}$. From this and (6.9), equation (4.14) can be rewritten as

$$\mathsf{S}^*_{jk} = \varepsilon\left(\delta_{jk} + \langle(\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_j \cdot (\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_k\rangle\right), \quad \mathsf{A}^*_{jk} = \langle \mathbf{A}(\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_j \cdot (\varepsilon\mathsf{I}+\mathbf{A})^{-1}\boldsymbol{g}_k\rangle, \tag{7.8}$$

where $\boldsymbol{g}_k = -\Gamma\mathsf{H}\boldsymbol{e}_k$. The integral representations for S^*_{jk} and A^*_{jk} in (7.7) follow from equations (3.6) and (7.8), 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 (7.7) by showing that the conditions of the spectral theorem of equation (3.6) are satisfied for the functionals in (7.8) and then employing these symmetries.

We first show that $\boldsymbol{g}_k \in \mathcal{F}$ for all $k = 1,\ldots,d$. Indeed, the orthogonality of the projection operators $\Gamma_W = \Gamma$ and Γ_0 defined in equation (4.11) implies that the vector field $\boldsymbol{g}_k(t,\cdot) = \Gamma\mathsf{H}(t,\cdot)\boldsymbol{e}_k$ is curl-free and mean-zero for each $t \in \mathcal{T}$ fixed, and by equation (6.3) we have $\|\boldsymbol{g}_k\| \le \|\mathsf{H}\| < \infty$. This and the periodicity of H implies that $\boldsymbol{g}_k(t,\cdot) \in \mathcal{H}_W$, and by Fubini's theorem [32] we have $\langle \boldsymbol{g}_k\rangle = 0$. By the uniform boundedness of Γ on $\mathcal{H}_\mathcal{V}$ and equation (6.3), we also have [32] that $\|\mathbf{T}\boldsymbol{g}_k\| = \|\mathbf{T}\Gamma\mathsf{H}\boldsymbol{e}_k\| = \|\Gamma\mathbf{T}\mathsf{H}\boldsymbol{e}_k\| \le \|\mathbf{T}\mathsf{H}\| < \infty$. 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 $k = 1,\ldots,d$.

Consider the representation for S^*_{jk} in (7.8) 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 $k = 1,\ldots,d$, 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}, $j,k = 1,\ldots,d$, in (7.7) follow from the second formula in (3.6) 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 $j,k = 1,\ldots,d$ [85]. We have therefore established that $\boldsymbol{g}_k \in \mathscr{D}(F)$ for all $k = 1,\ldots,d$.

Before we employ the symmetry $\langle \boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle \boldsymbol{\nabla}\chi_k \cdot \boldsymbol{\nabla}\chi_j\rangle$ to derive the integral representations for S^*_{kk} and S^*_{jk} in (7.7), we note that the condition $\mu^0_{kk} < \infty$ implies that $\boldsymbol{g}_k \in \mathscr{D}(F)$ for the function $F(z) = 1$. This leads to an explicit representation of the mass μ^0_{jk} in terms of Γ and H, and provides a bound for $|\mu^0_{jk}|$. Indeed, taking $F(z) = 1$ ($F(\mathbf{A}) = \mathsf{I}$), $\boldsymbol{\psi} = \boldsymbol{g}_j$, and $\boldsymbol{\varphi} = \boldsymbol{g}_k$ in the first formula of equation (3.6), the self-adjointness of Γ and $\Gamma^2 = \Gamma$ on $\mathcal{F}$ implies that

$$\mu^0_{jk} = \int_I \mathrm{d}\mu_{jk}(z) = \int_I \mathrm{d}\langle \mathbf{Q}(z)\boldsymbol{g}_j, \boldsymbol{g}_k\rangle = \langle \boldsymbol{g}_j, \boldsymbol{g}_k\rangle = \langle \Gamma\mathsf{H}\boldsymbol{e}_j \cdot \Gamma\mathsf{H}\boldsymbol{e}_k\rangle = \langle \mathsf{H}^T\Gamma\mathsf{H}\boldsymbol{e}_j \cdot \boldsymbol{e}_k\rangle. \tag{7.9}$$

This and equation (6.3) imply that $|\mu^0_{jk}| \le \|\mathsf{H}\|^2 < \infty$ for all $j,k = 1,\ldots,d$.

We now derive the integral representations for S^*_{kk} and S^*_{jk}, $j \ne k = 1,\ldots,d$, displayed in (7.7). For the function $F(z) = (\varepsilon+z)^{-1}$, we have established above that $\boldsymbol{g}_k \in \mathscr{D}(F)$ for all $k = 1,\ldots,d$, so that $\mathsf{S}^*_{jk} = \varepsilon(\delta_{jk} + \langle F(\mathbf{A})\boldsymbol{g}_j \cdot F(\mathbf{A})\boldsymbol{g}_k\rangle)$ is well defined in terms of a Radon–Stieltjes integral. Specifically, the second formula in equation (3.6) with $F(z) = G(z) = (\varepsilon+z)^{-1}$, $\boldsymbol{\psi} = \boldsymbol{g}_j$, $\boldsymbol{\varphi} = \boldsymbol{g}_k$, $\mathrm{d}\mu_{\psi\varphi}(z) := \mathrm{d}\mu_{jk}(z) = \mathrm{d}\langle \mathbf{Q}(z)\boldsymbol{g}_j \cdot \boldsymbol{g}_k\rangle = \mathrm{d}\langle \mathbf{Q}_2(\mathrm{Im}(z))\boldsymbol{g}_j \cdot \boldsymbol{g}_k\rangle$, and $z = \imath\lambda$ yields

$$\mathsf{S}^*_{jk}/\varepsilon - \delta_{jk} = \int_I \frac{\mathrm{d}\mu_{jk}(z)}{\overline{(\varepsilon+z)}(\varepsilon+z)} = \int_I \frac{\mathrm{d}\mu_{jk}(z)}{\varepsilon^2+|z|^2} = \int_{-\imath\infty}^{\imath\infty} \frac{\mathrm{d}\mu_{jk}(\mathrm{Im}(z))}{\varepsilon^2+|\mathrm{Im}(z)|^2} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}. \tag{7.10}$$

Equation (7.10) establishes the integral representation for S^*_{kk} in (7.7), since $\mu_{kk}(z) = \|\mathbf{Q}(z)\boldsymbol{g}_k\|^2$ is a positive function so that $\mathrm{Re}\,\mu_{kk}(z) = \mu_{kk}(z)$ and $\mathrm{d}\mu_{kk}(z) = \mathrm{d}\|\mathbf{Q}(z)\boldsymbol{g}_k\|^2$ is a *positive measure*. However for $j \ne k$, the function $\mu_{jk}(z) = \langle \mathbf{Q}(z)\boldsymbol{g}_j \cdot \boldsymbol{g}_k\rangle$ is complex-valued, with $\mu_{kj}(z) = \overline{\mu}_{jk}(z)$, so that $\mathrm{d}\mu_{jk}(z)$ is a *complex measure*. Since the vector field $\boldsymbol{\nabla}\chi_k$ is real-valued, the functional $\langle \boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle F(\mathbf{A})\boldsymbol{g}_j \cdot F(\mathbf{A})\boldsymbol{g}_k\rangle$ is also real-valued, which implies that the final integral in (7.10) must be representable in terms of a *signed measure* for $j \ne k$. The validity of this follows from the symmetry $\langle \boldsymbol{\nabla}\chi_j \cdot \boldsymbol{\nabla}\chi_k\rangle = \langle \boldsymbol{\nabla}\chi_k \cdot \boldsymbol{\nabla}\chi_j\rangle$, so that

$2\langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle=\langle\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle+\langle\boldsymbol{\nabla}\chi_k\cdot\boldsymbol{\nabla}\chi_j\rangle$. Therefore, since $\mu_{kj}(\lambda)=\overline{\mu}_{jk}(\lambda)$, by the linearity properties of Radon–Stieltjes integrals [85], for $j\neq k=1,\dots,d$, equation (7.10) becomes

$$\mathsf{S}^*_{jk}/\varepsilon-\delta_{jk}=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\mathrm{d}(\mu_{jk}(\lambda)+\overline{\mu}_{jk}(\lambda))}{\varepsilon^2+\lambda^2}=\int_{-\infty}^{\infty}\frac{\mathrm{dRe}\,\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\,, \tag{7.11}$$

which establishes the integral representation for S^*_{jk} in (7.7) for $j\neq k$. As anticipated, the integral representation for S^*_{jk} in equation (7.7) satisfies $\mathsf{S}^*_{kj}=\mathsf{S}^*_{jk}$, since $\mu_{kj}(\lambda)=\overline{\mu}_{jk}(\lambda)$ implies that $\mathrm{Re}\,\mu_{kj}(\lambda)=\mathrm{Re}\,\mu_{jk}(\lambda)$.

We now derive the integral representation for A^*_{jk}, $j\neq k=1,\dots,d$, displayed in equation (7.7). Consider the representation for A^*_{jk} in (7.8) and define the functions $F(z)=z(\varepsilon+z)^{-1}$ and $G(z)=(\varepsilon+z)^{-1}$ so that, formally, $\mathsf{A}^*_{jk}=\langle F(\mathbf{A})\boldsymbol{g}_j\cdot G(\mathbf{A})\boldsymbol{g}_k\rangle$. We have already established that $\boldsymbol{g}_k\in\mathscr{D}(G)$ for all $k=1,\dots,d$. Since $z=\imath\lambda$ and $\lambda,\varepsilon\in\mathbb{R}$, we have that the function $|F(z)|^2=\lambda^2(\varepsilon^2+\lambda^2)^{-1}<1$ for all $0<\varepsilon<\infty$. By equations (6.3) and (7.9), the positive measure $\mathrm{d}\mu_{kk}$ has bounded mass $\mu^0_{kk}\leq\|\mathsf{H}\|^2<\infty$, which implies that $F\in L^2(\mu_{kk})$ hence $\boldsymbol{g}_k\in\mathscr{D}(F)$ for all $k=1,\dots,d$. Consequently, the functional $\mathsf{A}^*_{jk}=\langle F(\mathbf{A})\boldsymbol{g}_j\cdot G(\mathbf{A})\boldsymbol{g}_k\rangle$ has a well defined meaning in terms of a Radon-Stieltjes integral. Specifically, the second formula in equation (3.6) with $F(z)=z(\varepsilon+z)^{-1}$, $G(z)=(\varepsilon+z)^{-1}$, $\boldsymbol{\psi}=\boldsymbol{g}_j$, $\boldsymbol{\varphi}=\boldsymbol{g}_k$, $\mathrm{d}\mu_{\psi\varphi}(z):=\mathrm{d}\mu_{jk}(z)$ defined as in equation (7.10), and $z=\imath\lambda$ yields

$$\mathsf{A}^*_{jk}=\int_I\frac{\overline{z}\,\mathrm{d}\mu_{jk}(z)}{\varepsilon^2+|z|^2}=\int_{-\imath\infty}^{\imath\infty}\frac{-\imath\,\mathrm{Im}(z)\mathrm{d}\mu_{jk}(\mathrm{Im}(z))}{\varepsilon^2+|\mathrm{Im}(z)|^2}=\int_{-\infty}^{\infty}\frac{-\imath\lambda\,\mathrm{d}\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\,. \tag{7.12}$$

Similar to the derivation of the integral representation for S^*_{jk} in (7.11) when $j\neq k$, we use that $\mathsf{A}^*_{jk}=\langle\mathbf{A}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle=\langle F(\mathbf{A})\boldsymbol{g}_j\cdot G(\mathbf{A})\boldsymbol{g}_k\rangle$ is real-valued. This implies that we have the symmetry $\langle\mathbf{A}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle=\langle\boldsymbol{\nabla}\chi_k\cdot\mathbf{A}\boldsymbol{\nabla}\chi_j\rangle$, so that $2\langle\mathbf{A}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle=\langle\mathbf{A}\boldsymbol{\nabla}\chi_j\cdot\boldsymbol{\nabla}\chi_k\rangle+\langle\boldsymbol{\nabla}\chi_k\cdot\mathbf{A}\boldsymbol{\nabla}\chi_j\rangle$. This, equation (7.12), $\mu_{kj}(z)=\overline{\mu}_{jk}(z)$, $z=\imath\lambda$, and the linearity properties of Radon–Stieltjes integrals [85] imply that

$$\mathsf{A}^*_{jk}=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\lambda\,\mathrm{d}(\imath\,[\overline{\mu}_{jk}(\lambda)-\mu_{jk}(\lambda)])}{\varepsilon^2+\lambda^2}=\int_{-\infty}^{\infty}\frac{\lambda\,\mathrm{dIm}\,\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\,, \tag{7.13}$$

which establishes the integral representation for A^*_{jk} in (7.7). As anticipated, the integral representation for A^*_{jk} in equation (7.7) satisfies $\mathsf{A}^*_{kj}=-\mathsf{A}^*_{jk}$, since $\mu_{kj}(\lambda)=\overline{\mu}_{jk}(\lambda)$ implies that $\mathrm{Im}\,\mu_{kj}(\lambda)=-\mathrm{Im}\,\mu_{jk}(\lambda)$. Moreover, since $\mu_{kk}(\lambda)$ is real-valued so that $\mathrm{Im}\,\mu_{kk}(\lambda)\equiv 0$, we also have $\mathsf{A}^*_{kk}=0$.

We have already discussed that the domain of integration I of the integral representations in (3.6) are determined by the spectrum $\Sigma(\mathbf{N})$ of the maximal normal operator $\mathbf{N}$. Hence, the domain of integration in equation (7.7) is determined by the spectrum $\Sigma(\mathbf{A})$ of the operator $\mathbf{A}$. Although, we were able to take $I\subseteq(-\infty,\infty)$ in (7.7) because of the properties of the functions $F(z)$, $G(z)$, and $\mu_{jk}(z)$ underlying these integral representations (see equations (7.10) and (7.12)). Since the spectral radius of the normal operator $\mathbf{A}$ is given by its norm $\|\mathbf{A}\|$ [77], I can be an unbounded set in the case of a time-dependent velocity field $\boldsymbol{u}$ and $I\subseteq[-\|\mathbf{A}\|,\|\mathbf{A}\|]$ with $\|\mathbf{A}\|\leq\|\mathsf{H}\|<\infty$ in the case of a time-independent velocity field. This concludes our proof of Theorem 7.1 $\square$.

7.2. General infinite dimensional setting - Sobolev. We now discuss an important corollary of Theorem 7.1 that provides integral representations for D^* and A^* in terms of an anti-symmetric operator A, which acts on *scalar-valued* functions. This formulation [70, 11] of the effective parameter problem for D^* has a more practical numerical implementation than that involving the operator $\mathbf{A}$, which acts on *vector-valued* functions, and will be used in Section 10 to compute the effective diffusivity tensor D^* for model flows. For the case of a time-independent, continuously differentiable velocity field $\boldsymbol{u}$, the operator A is compact on a Sobolev space $\mathscr{H}^1_{\mathcal{V}}$ [11], and a resolvent formula for χ_j involving A has led to [70] a discrete version of the integral representation for A^* displayed in (7.7). We now show that the conditions of Theorem 7.1 can be modified slightly to generalize this result for A^* to the case of a time-dependent velocity field $\boldsymbol{u}\in\otimes_{n=1}^d(\tilde{\mathscr{A}_{\mathcal{T}}}\otimes L^2(\mathcal{V}))$, as well as extending the result to D^*. The details are as follows.

Consider the Hilbert spaces $\mathscr{H}_{\mathcal{T}}$ and $\mathscr{H}_{\mathcal{V}}$ (over the complex field $\mathbb{C}$) of Lebesgue measurable, square integrable, scalar-valued functions, which are $\mathcal{T}$–periodic and $\mathcal{V}$–periodic, respectively, as well as their direct product $\mathscr{H}_{\mathcal{T}\mathcal{V}}$,

$$\mathscr{H}_{\mathcal{T}\mathcal{V}}=\mathscr{H}_{\mathcal{T}}\otimes\mathscr{H}_{\mathcal{V}},\quad\mathscr{H}_{\mathcal{T}}=\{f\in L^2(\mathcal{V})\mid f(0)=f(T)\},\quad\mathscr{H}_{\mathcal{V}}=\{f\in L^2(\mathcal{V})\mid f(0)=f(\boldsymbol{u})\}, \tag{7.14}$$

which are analogous to the Hilbert spaces $\mathcal{H}_\mathcal{T}$, $\mathcal{H}_\mathcal{V}$, and $\mathcal{H}_{\mathcal{T}\mathcal{V}}$ of vector-valued functions defined in equation (4.10). Denote by $\langle\cdot,\cdot\rangle$ the sesquilinear inner-product associated with the Hilbert space $\mathscr{H}_{\mathcal{T}\mathcal{V}}$, which is defined by $\langle f,h\rangle=\langle\overline{f}\,h\rangle$ with $\langle f,h\rangle=\overline{\langle h,f\rangle}$. Here, $\langle\cdot\rangle$ still denotes space-time averaging over $\mathcal{T}\times\mathcal{V}$ and we denote by $\|\cdot\|$ the norm induced by the $\mathscr{H}_{\mathcal{T}\mathcal{V}}$-inner-product. Analogous to the Hilbert space $\mathcal{H}_W\subset\mathcal{H}_\mathcal{V}$ defined in equation (4.11), we consider the Sobolev space $\mathscr{H}^1_\mathcal{V}\subset\mathscr{H}_\mathcal{V}$

$$\mathscr{H}^1_\mathcal{V}=\{f\in\mathscr{H}_\mathcal{V}\mid\langle|\boldsymbol{\nabla}f|^2\rangle_\mathcal{V}<\infty\},\tag{7.15}$$

which is also a Hilbert space [31]. Here, $\langle\cdot\rangle_\mathcal{V}$ denotes spatial averaging over $\mathcal{V}$. Finally, consider the function space $\mathscr{F}$ with inner-product $\langle\cdot,\cdot\rangle_1$

$$\mathscr{F}=\{f\in\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}\mid\langle f\rangle=0\},\qquad\langle f,g\rangle_1=\left\langle\overline{\boldsymbol{\nabla}f}\cdot\boldsymbol{\nabla}g\right\rangle,\tag{7.16}$$

which is analogous to $\mathcal{F}$ in (6.4) and involves the space $\tilde{\mathscr{A}_\mathcal{T}}$ of absolutely continuous, $\mathcal{T}$–periodic, scalar-valued functions defined in equation (3.11). We denote by $\|\cdot\|_1$ the norm induced by the $\mathscr{F}$-inner-product, where $h\in\mathscr{F}$ implies that $\|\partial_t h\|_1<\infty$ and $\|h\|_1<\infty$. In the case of a time-independent velocity field $\boldsymbol{u}$ we set $\tilde{\mathscr{A}_\mathcal{T}}=\emptyset$ in (4.3), so that $h\in\mathscr{F}$ implies $h\in\mathscr{H}^1_\mathcal{V}$ with $\langle h\rangle_\mathcal{V}=0$.

In terms of the $\mathscr{F}$-inner-product $\langle\cdot,\cdot\rangle_1$, the components S^*_{jk} and A^*_{jk}, $j,k=1,\ldots,d$, of the symmetric D^* and anti-symmetric A^* parts of the effective diffusivity tensor D^* are given by the following functionals [70],

$$\mathsf{S}^*_{jk}=\varepsilon(\delta_{jk}+\langle\chi_j,\chi_k\rangle_1),\qquad\mathsf{A}^*_{jk}=\langle A\chi_j,\chi_k\rangle_1,\quad A=\Delta^{-1}(\boldsymbol{u}\cdot\boldsymbol{\nabla}-\partial_t),\tag{7.17}$$

which are analogous to that in (4.14). The formulas for S^*_{jk} and A^*_{jk} in equation (4.4) follow [70] from $\mathsf{D}^*_{jk}=\varepsilon\delta_{jk}+\langle u_j\chi_k\rangle$ in (A.12) and the cell problem $-\varepsilon\Delta\chi_j-(\boldsymbol{u}\cdot\boldsymbol{\nabla}-\partial_t)\chi_j=u_j$ in equation (A.9):

$$\langle u_j\chi_k\rangle=\langle\Delta\Delta^{-1}u_j\chi_k\rangle=-\langle\boldsymbol{\nabla}\Delta^{-1}u_j\cdot\boldsymbol{\nabla}\chi_k\rangle=-\langle\Delta^{-1}u_j,\chi_k\rangle_1=\varepsilon\langle\chi_j,\chi_k\rangle_1+\langle A\chi_j,\chi_k\rangle_1,\tag{7.18}$$

where the periodicity of u_j and χ_k was used in the second equality. Applying the operator $-(\Delta^{-1})$ to both sides of equation (A.9), we obtain the following resolvent formula for χ_j involving A in (4.4), which is analogous to equation (6.9),

$$\chi_j=(\varepsilon+A)^{-1}g_j,\qquad g_j=(-\Delta)^{-1}u_j.\tag{7.19}$$

In equation (A.1) of Section A.1 we show that the incompressibility condition $\boldsymbol{\nabla}\cdot\boldsymbol{u}=0$ implies that the operator $(\Delta^{-1})(\boldsymbol{u}\cdot\boldsymbol{\nabla})$ is anti-symmetric on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$ [11]. Moreover, for $\boldsymbol{u}\in\otimes_{n=1}^d\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}_\mathcal{V}$, we also have that it is a bounded operator on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$. Indeed, since $\Delta=\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}$, we have

$$\|(\Delta^{-1})h\|_1^2=\langle\boldsymbol{\nabla}(\Delta^{-1})h\cdot\boldsymbol{\nabla}(\Delta^{-1})h\rangle=\langle[(-\Delta)^{-1}h]\,h\rangle,\quad\forall\,h\in\mathscr{F},\tag{7.20}$$

which implies that

$$\|(\Delta^{-1})(\boldsymbol{u}\cdot\boldsymbol{\nabla})h\|_1^2=|\langle[(\Delta^{-1})(\boldsymbol{u}\cdot\boldsymbol{\nabla})h]\,(\boldsymbol{u}\cdot\boldsymbol{\nabla})h\rangle|\le\|(\Delta^{-1})\|\,\|\boldsymbol{u}\|^2\|h\|_1^2<\infty,\tag{7.21}$$

where we have used the simplified notation $\|\boldsymbol{u}\|^2=\sum_j\|u_j\|^2$ and the fact [83] that (Δ^{-1}) is compact, hence bounded on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$. Since $(\Delta^{-1})(\boldsymbol{u}\cdot\boldsymbol{\nabla})$ is bounded anti-symmetric operator on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$, the operator $\imath(\Delta^{-1})(\boldsymbol{u}\cdot\boldsymbol{\nabla})$ is self-adjoint on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$. We have already established that $\imath\partial_t$ is a self-adjoint operator on the function space $\tilde{\mathscr{A}_\mathcal{T}}$ and that $\imath\partial_t$ and (Δ^{-1}) commute on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$, which implies that $\imath(\Delta^{-1})\partial_t$ is self-adjoint on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$. It is now clear that $M=-\imath A$, with $A=(\Delta^{-1})(\boldsymbol{u}\cdot\boldsymbol{\nabla}-\partial_t)$ is self-adjoint on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}^1_\mathcal{V}$. Finally, since an operator is self-adjoint if and only if it is a maximal normal operator [85], we have that A is a maximal normal operator on the function space $\mathscr{F}$. Using this alternative Hilbert space formulation of the effective parameter problem for D^*, we have the following corollary of Theorem 7.1.

COROLLARY 7.2. *Let $z=\imath\lambda$, $g_j=-(\Delta^{-1})u_j$ be defined as in* (4.7)*, and $Q(z)=Q_2(\mathrm{Im}(z))=Q_2(\lambda)$ be the complex resolution of the identity associated with the maximal anti-symmetric operator A defined in* (4.4)*, with domain $\mathscr{F}$ defined in* (4.3)*. Define the matrix-valued function $\boldsymbol{\mu}(\lambda)$ with complex-valued off-diagonal components $\mu_{jk}(\lambda)=\langle Q_2(\lambda)g_j,g_k\rangle_1$ for $j\neq k=1,\ldots,d$, with $\mu_{kj}=\overline{\mu}_{jk}$, and positive diagonal components $\mu_{kk}(\lambda)=\|Q_2(\lambda)g_k\|_1^2$. Moreover, consider the real-valued functions $\mathrm{Re}\,\mu_{jk}(\lambda)$ and $\mathrm{Im}\,\mu_{jk}(\lambda)$*

defined in (3.4)*. Corresponding to each of these functions of bounded variation, consider the associated Radon–Stieltjes measures* $\mathrm{d}\mu_{jk}(\lambda)$*,* $\mathrm{d}\mu_{kk}(\lambda)$*,* $\mathrm{dRe}\,\mu_{jk}(\lambda)$*, and* $\mathrm{dIm}\,\mu_{jk}(\lambda)$*. Then, for all* $0<\varepsilon<\infty$*, the Radon–Stieltjes integral representations in* (7.7) *hold for the functionals* S^*_{jk} *and* A^*_{jk} *defined in equation* (4.4)*. The domain of integration* I *is determined by the spectrum* $\Sigma(A)$ *of the operator* A*, where* $I\subseteq[-\|A\|,\|A\|]$ *and* $\|A\|\le\|(\Delta^{-1})\|\|\boldsymbol{u}\|\|\boldsymbol{\nabla}\|_1<\infty$ *in the case of a time-independent velocity field* $\boldsymbol{u}$*.*

Proof of Corollary 7.2. From equations (4.4) and (4.7) we have the following analogue of (7.8)

$$\mathsf{S}^*_{jk}=\varepsilon\left(\delta_{jk}+\langle(\varepsilon+A)^{-1}g_j,(\varepsilon+A)^{-1}g_k\rangle_1\right),\quad \mathsf{A}^*_{jk}=\langle A(\varepsilon+A)^{-1}g_j,(\varepsilon+A)^{-1}g_k\rangle_1, \tag{7.22}$$

where $g_j=-(\Delta^{-1})u_j$. By the proof of Theorem 7.1 and the properties $\chi_j, A\chi_j:\mathbb{R}W\mathbb{R}^d\to\mathbb{R}$, we need only to prove that $g_j\in\mathscr{F}$ for all $j=1,\ldots,d$. By equation (7.20) and $\boldsymbol{u}\in\otimes_{n=1}^d\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}_\mathcal{V}$, for each $t\in\mathcal{T}$ fixed, we have

$$\|g_j(t,\cdot)\|_1^2=|\langle[(\Delta^{-1})u_j(t,\cdot)]\,u_j(t,\cdot)\rangle|\le\|(\Delta^{-1})\|\,\|u_j(t,\cdot)\|^2<\infty, \tag{7.23}$$

Similarly, since the operators ∂_t and Δ^{-1} commute on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathscr{H}_\mathcal{V}$ and $u_j(\cdot,\boldsymbol{x})\in\tilde{\mathscr{A}_\mathcal{T}}$ for each $\boldsymbol{x}\in\mathcal{V}$ fixed, we have

$$\|\partial_t g_j(\cdot,\boldsymbol{x})\|_1=\|\partial_t(\Delta^{-1})u_j(\cdot,\boldsymbol{x})\|_1=\|(\Delta^{-1})\partial_t u_j(\cdot,\boldsymbol{x})\|_1\le\|\Delta^{-1}\|\,\|\partial_t u_j(\cdot,\boldsymbol{x})\|^2<\infty. \tag{7.24}$$

Finally, since $\boldsymbol{u}$ is mean-zero, we have that $\langle u_j(\cdot,\boldsymbol{x})\rangle=0$ for each $\boldsymbol{x}\in\mathcal{V}$ fixed. Therefore, by Fubini's theorem [32] we have that $\langle g_j\rangle=0$. Consequently, $g_j\in\mathscr{F}$ for all $j=1,\ldots,d$, which establishes that the integral representations in equation (7.7) hold for the functionals S^*_{jk} and A^*_{jk} defined in (4.4). Analogous to (7.9), by equation (7.20) the mass μ^0_{jk} of the associated measure $\mathrm{d}\mu_{jk}$ is given by

$$\mu^0_{jk}=\langle g_j,g_k\rangle_1=\langle[(-\Delta)^{-1}u_j]\,u_k\rangle, \tag{7.25}$$

which implies that $|\mu^0_{jk}|\le\|\Delta^{-1}\|\,\|u_j\|\,\|u_k\|<\infty$. The domain of integration I in (7.7) is determined by the spectrum $\Sigma(A)$ of the operator A, where $I\subseteq[-\|A\|,\|A\|]$ and $\|A\|\le\|(\Delta^{-1})\|\|\boldsymbol{u}\|\|\boldsymbol{\nabla}\|_1<\infty$ in the case of a time-independent velocity field $\boldsymbol{u}$. This concludes our proof of Corollary 7.2 □.

7.3. An isometric correspondence. A natural question to ask is the following. Is the formulation of the effective parameter problem described in Theorem 5.1 equivalent to that described in Corollary 7.2? The correspondence between the two formulations is one of isometry, and is summarized by the following theorem.

Theorem 7.3. *The function spaces* $\mathcal{F}$ *and* $\mathscr{F}$ *defined in equations* (6.4) *and* (4.3) *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* (6.9) *and* (4.4)*, 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 5.1 and Corollary 7.2 are equal,* $\mathrm{d}\langle Q_2(\lambda)g_j,g_k\rangle_1=\mathrm{d}\langle\mathbf{Q}_2(\lambda)\boldsymbol{g}_j,\boldsymbol{g}_k\rangle$*,* $j,k=1,\ldots,d$*, 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 7.3. We use the formula $\boldsymbol{u}=\boldsymbol{\nabla}\cdot\mathsf{H}$ displayed in equation (4.13) 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 (4.4) and (4.7) 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 $\Gamma=\boldsymbol{\nabla}(\Delta^{-1})\boldsymbol{\nabla}\cdot$ and the formulas $\boldsymbol{\nabla}\Delta^{-1}\partial_t=\boldsymbol{\Delta}^{-1}\mathbf{T}\boldsymbol{\nabla}$, $\boldsymbol{g}_j=-\Gamma\mathsf{H}\boldsymbol{e}_j$, and $\mathbf{A}=\Gamma\mathsf{H}-\boldsymbol{\Delta}^{-1}\mathbf{T}$ displayed in equations, (6.9), and (6.10), respectively, we have that

$$\boldsymbol{\nabla}A=[\Gamma\mathsf{H}-\boldsymbol{\Delta}^{-1}\mathbf{T}]\boldsymbol{\nabla}=\mathbf{A}\boldsymbol{\nabla},\qquad \boldsymbol{\nabla}g_j=\boldsymbol{g}_j. \tag{7.26}$$

Consequently, by applying the differential operator $\boldsymbol{\nabla}$ to both sides of the formula $(\varepsilon+A)\chi_j=g_j$ of (4.7), we obtain the formula $(\varepsilon\mathsf{I}+\mathbf{A})\boldsymbol{\nabla}\chi_j=\boldsymbol{g}_j$ of equation (6.9).

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 $\mathcal{H}_W$ and $\mathscr{H}^1_\mathcal{V}$ defined in equations (4.11) and (4.2), 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 $\Delta^{-1}\Delta f=f$ [83], which implies that $\Gamma \boldsymbol{\nabla} f = \boldsymbol{\nabla} f$ and $\|\boldsymbol{\nabla} f\|^2 = \langle \boldsymbol{\nabla} f \cdot \boldsymbol{\nabla} f \rangle = \|f\|_1^2 < \infty$. Consequently, for every $f \in \mathscr{H}_{\mathcal{V}}^1$ we have $\boldsymbol{\nabla} f \in \mathcal{H}_W$. Conversely, $\boldsymbol{\psi} \in \mathcal{H}_W$ implies that $\boldsymbol{\psi} = \Gamma \boldsymbol{\psi} = \boldsymbol{\nabla} f$, where we have defined the scalar-valued function $f = \Delta^{-1} \boldsymbol{\nabla} \cdot \boldsymbol{\psi}$. Since $\boldsymbol{\psi} = \boldsymbol{\nabla} f$, the $\mathscr{H}_{\mathcal{V}}^1$ norm of f satisfies $\|f\|_1^2 = \langle \boldsymbol{\psi} \cdot \boldsymbol{\psi} \rangle = \|\boldsymbol{\psi}\|^2 < \infty$ so that $f \in \mathscr{H}_{\mathcal{V}}^1$. 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 $\Gamma \boldsymbol{\psi} = \boldsymbol{\psi}$ implies that $\|f_1 - f_2\|_1 = \|\boldsymbol{\psi} - \boldsymbol{\psi}\| = 0$. Consequently, for every $\boldsymbol{\psi} \in \mathcal{H}_W$ there exists unique $f \in \mathscr{H}_{\mathcal{V}}^1$ such that $\boldsymbol{\psi} = \boldsymbol{\nabla} f$. In summary, the Hilbert spaces $\mathscr{H}_{\mathcal{V}}^1$ and $\mathcal{H}_W$ are in one-to-one isometric correspondence, which we denote by $\mathscr{H}_{\mathcal{V}}^1 \sim \mathcal{H}_W$. 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 [85]. 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 [85]. 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

$$\langle Xf, h\rangle_1 = \int_{-\infty}^{\infty} \lambda \, \mathrm{d}\langle Q(\lambda) f, h\rangle_1, \qquad \|Xf\|_1^2 = \int_{-\infty}^{\infty} \lambda^2 \, \mathrm{d}\|Q(\lambda) f\|_1^2, \tag{7.27}$$

where h is an arbitrary element in $\mathscr{F}$ [85]. 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 (7.12) and (7.13) shows that equation (3.7) holds under the mappings $X \mapsto A$, $\lambda \, \mathrm{d}\langle Q(\lambda) f, h\rangle_1 \mapsto \lambda \, \mathrm{dIm}\, \langle Q(\lambda) f, h\rangle_1$, 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 (7.26), 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 (7.26)

$$\|Af\|_1^2 = \langle Af, Af\rangle_1 = \langle \boldsymbol{\nabla} Af \cdot \boldsymbol{\nabla} Af\rangle = \langle \mathbf{A} \boldsymbol{\nabla} f \cdot \mathbf{A} \boldsymbol{\nabla} f\rangle = \|\mathbf{A} \boldsymbol{\nabla} f\|^2. \tag{7.28}$$

Consequently, from equation (3.7) we have

$$\int \lambda^2 \, \mathrm{d}\|Q_2(\lambda) f\|_1^2 = \int \lambda^2 \, \mathrm{d}\|\mathbf{Q}_2(\lambda) \boldsymbol{\nabla} f\|^2, \tag{7.29}$$

and the convergence of the left-hand-side of (7.29) 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 (7.26) then implies that

$$\|\mathbf{A} \boldsymbol{\psi}\|^2 = \langle \mathbf{A} \boldsymbol{\nabla} f, \mathbf{A} \boldsymbol{\nabla} f\rangle = \langle \boldsymbol{\nabla} Af, \boldsymbol{\nabla} Af\rangle = \langle Af, Af\rangle_1 = \|Af\|_1^2. \tag{7.30}$$

Again, equation (3.7) implies that (7.29) holds, and the convergence of the right-hand-side of (7.29) 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 (7.29) and the linearity properties of Radon–Stieltjes integrals [85], we have that

$$0 = \int_{-\infty}^{\infty} \lambda^2 \, \mathrm{d}(\|Q_2(\lambda) f\|_1^2 - \|\mathbf{Q}_2(\lambda) \boldsymbol{\nabla} f\|^2) = \int_{-\infty}^{\infty} \lambda^2 \, \mathrm{d}(\langle [\boldsymbol{\nabla} Q_2(\lambda) - \mathbf{Q}_2(\lambda) \boldsymbol{\nabla}] f \cdot \boldsymbol{\nabla} f\rangle). \tag{7.31}$$

Equation (7.31) 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 [85], 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 (7.31) holds and implies equation (7.29). The correspondence $D(A) \sim D(\mathbf{A})$ and equation (3.7) 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 5.1 and Corollary 7.2 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 $j,k = 1,\dots,d$. This concludes our proof of Theorem 7.3 $\square$.

8. Cell flows and Fourier methods. In this section we discuss how Fourier methods can be employed to calculate the symmetric D^* and anti-symmetric A^* parts of the effective diffusivity tensor D^* for a large class of velocity fields $\boldsymbol{u}$. It is more natural to focus on the approach discussed in Section 7.2, as opposed to that of Section 7.1, as the underlying operators are *sparse* (infinite) matrices in Fourier space and the velocity field $\boldsymbol{u}$ appears naturally, as opposed to the stream matrix H. Our use of Fourier methods in this section is two-fold. In Section 8.1, we will apply them to the eigenvalue problem $A\varphi_n = \imath\lambda_n\varphi_n$ to explicitely calculate the discrete component of the spectral measure $\mathrm{d}\boldsymbol{\mu}(\lambda)$ underlying the integral representations for D^* and A^* displayed in equation (A.31).

8.1. Spectral methods. In this section, we use Fourier and spectral methods in concert to obtain explicit representations for the spectral weights $\overline{\langle\varphi_n, g_j\rangle}_1\langle\varphi_n, g_k\rangle_1$, $n \in \mathbb{Z}$, $j,k = 1,\dots,d$, at the heart of the integral representations for D^* and A^*, displayed in equation (A.31), for a large class of velocity fields $\boldsymbol{u}$. In particuar, we consider velocity fields $\boldsymbol{u}$ with components u_j, $j = 1,\dots,d$, which are representable by a *finite* number of Fourier modes. More specifically, we consider $\boldsymbol{u} \in \mathcal{U}$, where

$$(8.1)\qquad \mathcal{U} = \otimes_{j=1}^d \mathcal{U}_j, \qquad \mathcal{U}_j = \Big\{u_j \in \mathscr{H}^1 : u_j = \sum_{(\ell,\boldsymbol{k})\in I_M^{d+1}} b_{\ell,\boldsymbol{k}}^j \,\mathrm{e}^{\imath(\ell t + \boldsymbol{k}\cdot\boldsymbol{x})}\Big\}, \quad b_{\ell,\boldsymbol{k}}^j = \big\langle u_j(t,\boldsymbol{x}), \mathrm{e}^{\imath(\ell t + \boldsymbol{k}\cdot\boldsymbol{x})}\big\rangle_2,$$

where $\mathscr{H}^1$ is defined in equation (A.19), $\boldsymbol{k} = (k_1,\dots,k_d)$, and the summation index set I_M^{d+1} is defined as $I_M^{d+1} = \{\boldsymbol{q} \in \mathbb{Z}^{d+1} : -M \le q_i \le M,\ M \in \mathbb{N}\}$. It is well known that $\mathcal{U}$ is dense in $\mathscr{H}^1$ [32].

Consider the eigenvalue problem $A\varphi_n = \imath\lambda_n\varphi_n$, $\lambda_n \in \mathbb{R}$, $n \in \mathbb{Z}$, involving the integro-differential operator $A = \Delta^{-1}(\boldsymbol{u}\cdot\boldsymbol{\nabla} - \partial_t)$ defined in equation (4.4). This equation may be rewritten as

$$(8.2)\qquad (\boldsymbol{u}\cdot\boldsymbol{\nabla} - \partial_t)\varphi_n = \imath\lambda_n\Delta\varphi_n.$$

Since $\varphi_n \in \mathscr{F} \subset \mathscr{H}^1$ and $\{\mathrm{e}^{\imath(\ell t + \boldsymbol{k}\cdot\boldsymbol{x})} : \ell \in \mathbb{Z},\ \boldsymbol{k} \in \mathbb{Z}^d\}$ is an orthonormal basis in $\mathscr{H}^1$ [32] we may represent φ_n by

$$(8.3)\qquad \varphi_n(t,\boldsymbol{x}) = \sum_{(\ell,\boldsymbol{k})\in\mathbb{Z}^{d+1}} a_{\ell,\boldsymbol{k}}^n \,\mathrm{e}^{\imath(\ell t + \boldsymbol{k}\cdot\boldsymbol{x})},$$

Inserting this into equation (8.2) and denoting $\boldsymbol{b}_{\ell',\boldsymbol{k}} = \big(b_{\ell',\boldsymbol{k}'}^1,\dots,b_{\ell',\boldsymbol{k}'}^d\big)$ the Fourier coefficients of $\boldsymbol{u} = (u_1,\dots,u_d)$ in (8.1) yields

$$(8.4)\qquad \sum_{(\ell,\boldsymbol{k})\in\mathbb{Z}^{d+1}} a_{\ell,\boldsymbol{k}}^n \,\mathrm{e}^{\imath(\ell t + \boldsymbol{k}\cdot\boldsymbol{x})}\left(\sum_{(\ell',\boldsymbol{k}')\in I_M^{d+1}} \mathrm{e}^{\imath(\ell' t + \boldsymbol{k}'\cdot\boldsymbol{x})}\,\big[\boldsymbol{b}_{\ell',\boldsymbol{k}'}\cdot\imath\boldsymbol{k}\big] - \imath\ell + \imath\lambda_n|\boldsymbol{k}|^2\right) = 0.$$

Comining, removing the common factor $\imath$, and renumbering the summation involving $\mathrm{e}^{\imath((\ell+\ell')t + (\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{x})}$ in (8.4) yields,

$$(8.5)\qquad \sum_{(\ell,\boldsymbol{k})\in\mathbb{Z}^{d+1}} \mathrm{e}^{\imath(\ell t + \boldsymbol{k}\cdot\boldsymbol{x})}\left(\sum_{(\ell',\boldsymbol{k}')\in I_M^{d+1}} \big[\boldsymbol{b}_{\ell',\boldsymbol{k}'}\cdot(\boldsymbol{k}-\boldsymbol{k}')\big]\, a_{\ell-\ell',\boldsymbol{k}-\boldsymbol{k}'}^n - \ell a_{\ell,\boldsymbol{k}}^n + \lambda_n|\boldsymbol{k}|^2 a_{\ell,\boldsymbol{k}}^n\right) = 0.$$

Since the orthogonal set $\{\mathrm{e}^{\imath(\ell t + \boldsymbol{k}\cdot\boldsymbol{x})} : \ell \in \mathbb{Z},\ \boldsymbol{k} \in \mathbb{Z}^d\}$ is complete, we have [85, 46] from (8.5) that

$$(8.6)\qquad \sum_{(\ell',\boldsymbol{k}')\in I_M^{d+1}} \big[\boldsymbol{b}_{\ell',\boldsymbol{k}'}\cdot(\boldsymbol{k}-\boldsymbol{k}')\big]\, a_{\ell-\ell',\boldsymbol{k}-\boldsymbol{k}'}^n - \ell a_{\ell,\boldsymbol{k}}^n = -\lambda_n|\boldsymbol{k}|^2 a_{\ell,\boldsymbol{k}}^n.$$

Equation (8.6) defines a matrix equation as follows. Define the bijective linear mapping Θ of I_M^{d+1} to $I_M=\{q\in\mathbb{Z}:1\le q_i\le(2M+1)^d,\ M\in\mathbb{N}\}$, $\Theta:I_M^d\mapsto I_M$,

$$\Theta(\ell,\boldsymbol{k})=1+\sum_{j=1}^{d}(M+k_j)(2M+1)^{j-1}+(M+\ell)(2M+1)^d. \tag{8.7}$$

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

$$\left\langle \mathrm{e}^{\imath(\ell t+\boldsymbol{k}\cdot\boldsymbol{x})},\ \mathrm{e}^{\imath(\ell' t+\boldsymbol{k}'\cdot\boldsymbol{x})}\right\rangle_2=\delta_{\ell,\ell'}\prod_{j=1}^{d}\delta_{k_j,k_j'} \tag{8.8}$$

provides a convenient series representation for the spectral weights $\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1$ underlying the integral representations for D^* and A^* displayed in equation (A.31). This representation follows from equations (A.35), (8.3), and (8.8)

$$\langle\varphi_n,g_j\rangle_1=\langle\varphi_n,u_j\rangle_2=\sum_{(\ell',\boldsymbol{k}')\in I_M^{d+1}}\overline{a^n_{\ell',\boldsymbol{k}'}}\,b^j_{\ell',\boldsymbol{k}'} \tag{8.9}$$

We now discuss how the orthogonality condition $\langle\varphi_n,\varphi_i\rangle_1=\delta_{li}$ in (A.20) is transformed by the Fourier expansion of the eigenfunctions $\varphi_n(t,\boldsymbol{x})$. This expansion of $\varphi_n(t,\boldsymbol{x})$ implies that for $\boldsymbol{\nabla}\varphi_n(t,\boldsymbol{x})$ as follows

$$\varphi_n(t,\boldsymbol{x})=\sum_{\ell,m,n}a^l_{\ell,m,n}\mathrm{e}^{\imath(\ell t+mx+ny)}\Rightarrow\boldsymbol{\nabla}\varphi_n(t,\boldsymbol{x})=\sum_{\ell,m,n}a^l_{\ell,m,n}\,(m,n)\,\mathrm{e}^{\imath(\ell t+mx+ny)}. \tag{8.10}$$

where $\langle\cdot,\cdot\rangle_2$ denotes the $L^2(\mathcal{T}\times\mathcal{V})$ inner-product, and that $\langle\cdot\rangle$ denotes space-time averaging. Consequently, we have that the orthogonality relation in (A.20) is transformed to

$$\delta_{li}=\langle\boldsymbol{\nabla}\varphi_n\cdot\boldsymbol{\nabla}\varphi_i\rangle=\sum_{\ell,m,n}(m^2+n^2)\,\overline{a^l_{\ell,m,n}}\,a^i_{\ell,m,n} \tag{8.11}$$

Recall that $\sum_i i^{-p}$ converges for all $p>1$. From this and equation (8.11) we see that the square modulus of the Fourier coefficients $a^l_{0,m,n}$ must have the asymptotic behavior $|a^l_{0,m,n}|^2\sim o((m^2+n^2)^{-3/2})$ as $m,n\to 1\infty$. Since $\varphi_n(\cdot,\boldsymbol{x})\in\tilde{\mathscr{A}}_{\mathcal{T}}(\mathcal{T})$, i.e. $\partial_t\varphi_n(\cdot,\boldsymbol{x})\in L^2(\mathcal{T})$, we also have $|a^l_{\ell,m,n}|^2\sim o(\ell^{-3})$ as $\ell\to 1\infty$. Since $\partial_t\boldsymbol{\nabla}\varphi_n\in L^2(\mathcal{T}\times\mathcal{V})$ we may generalize both of these statements by the following

$$|a^l_{\ell,m,n}|^2\sim o(\ell^{-3}(m^2+n^2)^{-3/2}),\ \text{as}\ \ \ell,m,n\to 1\infty. \tag{8.12}$$

9. Numerical Results. Consider the eigenvalue problem $A\varphi_n=\imath\lambda_n\varphi_n$, $\imath=\sqrt{-1}$, $\lambda_n\in\mathbb{R}$, $l=1,2,3,\ldots$, involving the integro-differential operator $A=(-\Delta)^{-1}(\partial_t+\boldsymbol{u}\cdot\boldsymbol{\nabla})$, introduced in equation (45) of our (attached) effective-diffusivity paper, with $\boldsymbol{u}\mapsto-\boldsymbol{u}$. Here A is an anti-symmetric (normal) operator and the incompressible velocity field $\boldsymbol{u}(t,\boldsymbol{x})$ is given in equation (9.13) above. The equation $A\varphi_n=\imath\lambda_n\varphi_n$ may be rewritten as

$$(\partial_t+\boldsymbol{u}\cdot\boldsymbol{\nabla})\varphi_n=-\imath\lambda_n\Delta\varphi_n. \tag{9.1}$$

The eigenfunctions φ_n satisfy the following orthogonality condition in (A.20)

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

$$\mathscr{F}=\{f\in\tilde{\mathscr{A}}_{\mathcal{T}}(\mathcal{T})\otimes\mathscr{H}^1(\mathcal{V})\,|\,\langle f\rangle=0\ \text{and is periodic on}\ \mathcal{T}\times\mathcal{V}\}. \tag{9.2}$$

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

$$\varphi_n(t,\boldsymbol{x})=\sum_{\ell}\varphi^l_{\ell}(\boldsymbol{x})\,\mathrm{e}^{\imath\ell t}, \tag{9.3}$$

where $\varphi_\ell^l \in \mathscr{H}^1(\mathcal{V})$. Write $\cos t = (\mathrm{e}^{\imath t} + \mathrm{e}^{-\imath t})/2$ and insert this and (9.3) into equation (9.1), yielding

$$\sum_\ell (\imath\ell + \boldsymbol{u}_1 \cdot \boldsymbol{\nabla} + \imath\lambda_n \Delta)\varphi_\ell^l(\boldsymbol{x})\mathrm{e}^{\imath\ell t} + \frac{\delta}{2}\sum_\ell (\mathrm{e}^{\imath(\ell+1)t} + \mathrm{e}^{\imath(\ell-1)t})\, \boldsymbol{u}_2 \cdot \boldsymbol{\nabla}\varphi_\ell^l(\boldsymbol{x}) = 0, \tag{9.4}$$

or:

$$\sum_\ell \left[(\imath\ell + \boldsymbol{u}_1 \cdot \boldsymbol{\nabla} + \imath\lambda_n \Delta)\varphi_\ell^l(\boldsymbol{x}) + \frac{\delta}{2}\boldsymbol{u}_2 \cdot \boldsymbol{\nabla}(\varphi_{\ell-1}^l(\boldsymbol{x}) + \varphi_{\ell+1}^l(\boldsymbol{x}))\right] \mathrm{e}^{\imath\ell t} = 0. \tag{9.5}$$

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

$$(\imath\ell + \boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi_\ell^l(\boldsymbol{x}) + \frac{\delta}{2}\boldsymbol{u}_2 \cdot \boldsymbol{\nabla}(\varphi_{\ell-1}^l(\boldsymbol{x}) + \varphi_{\ell+1}^l(\boldsymbol{x})) = -\imath\lambda_n\Delta\varphi_\ell^l(\boldsymbol{x}). \tag{9.6}$$

The system of partial differential equations in (9.6) 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

$$\begin{aligned}(\boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi_\ell^l(\boldsymbol{x}) &= \cos y\, \partial_x \varphi_\ell^l(\boldsymbol{x}) + \cos x\, \partial_y \varphi_\ell^l(\boldsymbol{x}) \\ (\boldsymbol{u}_2 \cdot \boldsymbol{\nabla})\varphi_\ell^l(\boldsymbol{x}) &= \sin y\, \partial_x \varphi_\ell^l(\boldsymbol{x}) + \sin x\, \partial_y \varphi_\ell^l(\boldsymbol{x})\end{aligned} \tag{9.7}$$

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

$$\varphi_\ell^l(\boldsymbol{x}) = \sum_{m,n} a_{\ell,m,n}^l\, \mathrm{e}^{\imath(mx+ny)} \tag{9.8}$$

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 (9.8) into equation (9.7), yielding

$$\begin{aligned}&(\boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi_\ell^l \\ &\quad = \frac{1}{2}\sum_{m,n} a_{\ell,m,n}^l \left[\imath m\, \mathrm{e}^{\imath m x}(\mathrm{e}^{\imath(n+1)y} + \mathrm{e}^{\imath(n-1)y}) + \imath n\, \mathrm{e}^{\imath n y}(\mathrm{e}^{\imath(m+1)x} + \mathrm{e}^{\imath(m-1)x})\right] \\ &(\boldsymbol{u}_2 \cdot \boldsymbol{\nabla})\varphi_\ell^l \\ &\quad = \frac{1}{2\imath}\sum_{m,n} a_{\ell,m,n}^l \left[\imath m\, \mathrm{e}^{\imath m x}(\mathrm{e}^{\imath(n+1)y} - \mathrm{e}^{\imath(n-1)y}) + \imath n\, \mathrm{e}^{\imath n y}(\mathrm{e}^{\imath(m+1)x} - \mathrm{e}^{\imath(m-1)x})\right]\end{aligned} \tag{9.9}$$

or:

$$\begin{aligned}(\boldsymbol{u}_1 \cdot \boldsymbol{\nabla})\varphi_\ell^l &= \frac{\imath}{2}\sum_{m,n}[m(a_{\ell,m,n-1}^l + a_{\ell,m,n+1}^l) + n(a_{\ell,m-1,n}^l + a_{\ell,m+1,n}^l)]\mathrm{e}^{\imath(mx+ny)} \\ (\boldsymbol{u}_2 \cdot \boldsymbol{\nabla})\varphi_\ell^l &= \frac{1}{2}\sum_{m,n}[m(a_{\ell,m,n-1}^l - a_{\ell,m,n+1}^l) + n(a_{\ell,m-1,n}^l - a_{\ell,m+1,n}^l)]\mathrm{e}^{\imath(mx+ny)}.\end{aligned} \tag{9.10}$$

We also have

$$-\Delta\varphi_\ell^l = \sum_{m,n} a_{\ell,m,n}^l (m^2 + n^2)\mathrm{e}^{\imath(mx+ny)} \tag{9.11}$$

By the completeness of the orthogonal set $\{\mathrm{e}^{\imath(mx+ny)}\}$, inserting equations (9.10) and (9.11) into equation (9.6) yields

$$\begin{aligned}\imath\ell\, a_{\ell,m,n}^l &+ \frac{\imath}{2}[m(a_{\ell,m,n-1}^l + a_{\ell,m,n+1}^l) + n(a_{\ell,m-1,n}^l + a_{\ell,m+1,n}^l)] \\ &+ \frac{\delta}{4}[m(a_{\ell-1,m,n-1}^l - a_{\ell-1,m,n+1}^l) + n(a_{\ell-1,m-1,n}^l - a_{\ell-1,m+1,n}^l) \\ &\quad + m(a_{\ell+1,m,n-1}^l - a_{\ell+1,m,n+1}^l) + n(a_{\ell+1,m-1,n}^l - a_{\ell+1,m+1,n}^l)] \\ &= \imath\lambda_n(m^2 + n^2)a_{\ell,m,n}^l,\end{aligned} \tag{9.12}$$

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 (9.13) and the Fourier expansion of the eigenfunctions φ_n in (8.10) allow the spectral weights $\langle\varphi_n,g_j\rangle$ in equation (A.31) to be given in terms of the Fourier coefficients $a^l_{\ell,m,n}$ for the reduced index set $\ell,m,n\in\{-1,0,1\}$.

$$\boldsymbol{u}(t,\boldsymbol{x})=(\cos y,\cos x)+\delta\cos t\,(\sin y,\sin x):=\boldsymbol{u}_1(\boldsymbol{x})+\delta\cos t\;\boldsymbol{u}_2(\boldsymbol{x}). \tag{9.13}$$

Writing $\cos x=(\mathrm{e}^{\imath x}+\mathrm{e}^{-\imath x})/2$ and $\sin x=(\mathrm{e}^{\imath x}-\mathrm{e}^{-\imath x})/(2\imath)$, for example, from equation (9.13) we have that

$$\begin{aligned} u_1(t,x,y)&=\cos y+\cos t\sin y\\ &=\frac{1}{2}\left(\mathrm{e}^{\imath y}+\mathrm{e}^{-\imath y}\right)+\frac{1}{4\imath}\left(\mathrm{e}^{\imath t}+\mathrm{e}^{-\imath t}\right)(\mathrm{e}^{\imath y}-\mathrm{e}^{-\imath y})\\ &=\frac{1}{2}\left(\mathrm{e}^{\imath y}+\mathrm{e}^{-\imath y}\right)+\frac{1}{4\imath}\left(\mathrm{e}^{\imath(t+y)}-\mathrm{e}^{\imath(t-y)}+\mathrm{e}^{\imath(-t+y)}-\mathrm{e}^{\imath(-t-y)}\right), \end{aligned} \tag{9.14}$$

and $u_2(t,x,y)=u_1(t,y,x)$. This, equation (A.35), and the orthogonality relation in (8.8) imply that

$$\begin{aligned} \langle\varphi_n,g_1\rangle_1&=\frac{1}{2}\left(a^l_{0,0,1}+a^l_{0,0,-1}\right)+\frac{1}{4\imath}\left(a^l_{1,0,1}-a^l_{1,0,-1}+a^l_{-1,0,1}-a^l_{-1,0,-1}\right)\\ \langle\varphi_n,g_2\rangle_1&=\frac{1}{2}\left(a^l_{0,1,0}+a^l_{0,-1,0}\right)+\frac{1}{4\imath}\left(a^l_{1,1,0}-a^l_{1,-1,0}+a^l_{-1,1,0}-a^l_{-1,-1,0}\right) \end{aligned} \tag{9.15}$$

Since $\boldsymbol{u}_i$ is incompressible, there exists an anti-symmetric matrix H_i such that $\boldsymbol{u}_i=\boldsymbol{\nabla}\cdot\mathsf{H}_i$. This allows us to write $\boldsymbol{u}_i\cdot\boldsymbol{\nabla}=\boldsymbol{\nabla}\cdot\mathsf{H}_i\boldsymbol{\nabla}$, which is an anti-symmetric operator. When $\delta=0$, the velocity field $\boldsymbol{u}$ is time-independent and the operator A, which arises from the cell problem, becomes $A=(-\Delta)^{-1}(\boldsymbol{u}_1\cdot\boldsymbol{\nabla})$. In this case, the eigenvalue problem in (9.1) becomes

$$\boldsymbol{\nabla}\cdot\mathsf{H}_1\boldsymbol{\nabla}\varphi=\lambda\Delta\varphi. \tag{9.16}$$

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

9.1. Matrix representations of the eigenvalue problem. In the *time-independent case*, where $\delta=0$ in the velocity field of equation (9.13), the system of equations in (9.12) corresponding to the eigenvalue problem becomes

$$m(a_{m,n-1}+a_{m,n+1})+n(a_{m-1,n}+a_{m+1,n})=2\lambda(m^2+n^2)a_{m,n},\quad m,n\in\mathbb{Z}, \tag{9.17}$$

where, for simplicity, we have dropped the super-script and sub-script, and have written $a_{m,n}=a^l_{m,n}$ and $\lambda=\lambda_n$. When the indices in equation (9.17) are restricted to be finite, $-M\le m,n\le M$ say, and suitable boundary conditions are imposed, it can be written in matrix form

$$B\boldsymbol{a}_l=2\lambda_nC\boldsymbol{a}_l, \tag{9.18}$$

where B and C are $(2M+1)^2W(2M+1)^2$ symmetric matrices and $l=1,\ldots,(2M+1)^2$. More specifically, B is real-symmetric and C is real-diagonal positive-semi-definite. Equation (9.18) is a generalized eigenvalue problem. Since B and C are symmetric matrices, the generalized eigenvalues are real $\lambda_n\in\mathbb{R}$ and the eigen-vectors $\boldsymbol{a}_l$ – consisting of the Fourier coefficients for φ_n – satisfy the orthogonality condition

$$\boldsymbol{a}_j^T C\boldsymbol{a}_k=\delta_{jk}. \tag{9.19}$$

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

In the *time-dependent* case, where $\delta \neq 0$ in the velocity field of equation (9.13), slightly manipulating equation (9.12) yields

$$\begin{aligned} 4\ell\, a_{\ell,m,n} &+ 2[m(a_{\ell,m,n-1} + a_{\ell,m,n+1}) + n(a_{\ell,m-1,n} + a_{\ell,m+1,n})] \\ &-\imath\delta[m(a_{\ell-1,m,n-1} - a_{\ell-1,m,n+1} + a_{\ell+1,m,n-1} - a_{\ell+1,m,n+1}) \\ &\quad + n(a_{\ell-1,m-1,n} - a_{\ell-1,m+1,n} + a_{\ell+1,m-1,n} - a_{\ell+1,m+1,n})] \\ &= 4\lambda(m^2+n^2)a_{\ell,m,n}. \end{aligned} \tag{9.20}$$

By restricting the indices, $-M \leq l, m, n \leq M$, in equation (9.20) and imposing suitable boundary conditions, it can also be written as the generalized eigenvalue problem of equations (9.18) and (9.19), where B and C are $(2M+1)^3 W (2M+1)^3$ symmetric matrices. More specifically, B is Hermitian-symmetric and C is real-diagonal. The rows and columns of B and C, corresponding to the $a_{0,0,0}$ component of $\boldsymbol{a}$, consist entirely of zero elements. Therefore, without loss of generality, they can be removed from the generalized eigenvalue problem, making the matrix C positive-definite.

10. Numerical Results. In this section we discuss the numerical implementation of the integral representations in equation (**??**), involving the signed, discrete measures displayed in (**??**). In particular, we directly compute the spectral measure $\mathrm{d}\boldsymbol{\mu}(\lambda)$ associated with discretizations of velocity fields $\boldsymbol{u}$ for model flows, to compute the symmetric D^* and anti-symmetric A^* parts of the associated effective diffusivity tensor D^*. We explore the numerical implementation of the different formulations of the effective parameter problem, described by Corollary 7.2 and Theorem 7.1 which involve the anti-symmetric operators A and $\mathbf{A}$, respectively. This analysis demonstrates that formulation described by Corollary 7.2 provides a more practical numerical implementation than that described in Theorem 7.1, as A is a *sparse* matrix of size N, say, and $\mathbf{A}$ is a *full* matrix of size dN.

Appendix A. Appendix.

A.1. Antisymmetry. In this section we show that the operator $A = (-\Delta)^{-1}(\partial_t - \boldsymbol{u}\cdot\boldsymbol{\nabla})$ defined in equation (4.4) is *antisymmetric* on the function space $\mathscr{F}$ defined in (4.3). We first show that the incompressibility condition $\boldsymbol{\nabla}\cdot\boldsymbol{u} = 0$ implies that the operator $(\Delta^{-1})(\boldsymbol{u}\cdot\boldsymbol{\nabla})$ is antisymmetric [11] on the Sobelov space $\mathscr{H}^1_{\mathcal{V}}$ defined in equation (4.2). Indeed, since $\Delta = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}$ and (Δ^{-1}) is self-adjoint [83] on $\mathscr{H}^1_{\mathcal{V}}$, for $f, h \in \mathscr{H}^1_{\mathcal{V}}$ we have

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

We now show that the operator $(-\Delta)^{-1}\partial_t$ is skew-adjoint on $\mathscr{F}$. For $f \in \mathscr{F}$ we have $f(\cdot, \boldsymbol{x}) \in \tilde{\mathscr{A}_{\mathcal{T}}}$ for all $\boldsymbol{x} \in \mathcal{V}$ and $f(t,\cdot) \in \mathscr{H}^1_{\mathcal{V}}$ for every $t \in \mathcal{T}$. Moreover, since $\mathscr{H}^1_{\mathcal{V}} \subset L^2(\mathcal{V})$ and $(-\Delta)^{-1}$ is a bounded Hilbert-Schmidt integral operator on $L^2(\mathcal{V})$ [83], Theorem 2.27 of [32] establishes that the operators $(-\Delta)^{-1}$ and ∂_t commute on $\mathscr{F}$. Consequently, since $(-\Delta)^{-1}$ is self-adjoint on $L^2(\mathcal{V})$ and ∂_t is skew-adjoint on $\tilde{\mathscr{A}_{\mathcal{T}}}$, the operator $(-\Delta)^{-1}\partial_t$ is skew-adjoint on $\mathscr{F}$. It follows that the operator $A = (-\Delta)^{-1}(\partial_t - \boldsymbol{u}\cdot\boldsymbol{\nabla})$ is *antisymmetric* on $\mathscr{F}$ $\square$.

A.2. Multiple scale method. In this section we provide the details of the multiple scale method [59, 68, 69, 8] which leads to equations (2.3)–(4.14). We assume that equation (2.1) has already been non-dimensionalized so that $\kappa_0 \mapsto \varepsilon$ and $\boldsymbol{u} \mapsto \boldsymbol{u}$. The key assumption of the method is that the initial density ϕ_0 in (2.1) is slowly varying relative to the velocity field $\boldsymbol{u}$, which introduces a small parameter $\delta \ll 1$ such that

$$\phi(0, \boldsymbol{x}) = \phi_0(\delta \boldsymbol{x}). \tag{A.2}$$

The variable changes $\boldsymbol{x} \mapsto \boldsymbol{y} = \boldsymbol{x}/\delta$ and $t \mapsto \tau = t/\delta^2$, along with equations (**??**) and (A.2), transforms equation (2.1) into [59]

$$\partial_t \phi^\delta(t, \boldsymbol{x}) = \varepsilon \Delta \phi^\delta(t, \boldsymbol{x}) + \delta^{-1} \boldsymbol{u}(\tau, \boldsymbol{y}) \cdot \boldsymbol{\nabla} \phi^\delta(t, \boldsymbol{x}), \quad \phi^\delta(0, \boldsymbol{x}) = \phi_0(\boldsymbol{x}). \tag{A.3}$$

We now expand ϕ^δ in powers of δ [59]

$$\phi^\delta(t, \boldsymbol{x}) = \bar{\phi}(t, \boldsymbol{x}) + \delta \phi^{(1)}(t, \boldsymbol{x}, \tau, \boldsymbol{y}) + \delta^2 \phi^{(2)}(t, \boldsymbol{x}, \tau, \boldsymbol{y}) + \cdots. \tag{A.4}$$

Writing

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

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

$$\begin{aligned} \partial_t \phi^\delta &= \delta^{-2}[\partial_\tau \bar{\phi}] + \delta^{-1}[\partial_\tau \phi^{(1)}] + \delta^0[\partial_t \bar{\phi} + \partial_\tau \phi^{(2)}] + O(\delta), \\ \boldsymbol{\nabla} \phi^\delta &= \delta^{-2}[0] + \delta^{-1}[\boldsymbol{\nabla}_y \bar{\phi}] + \delta^0[\boldsymbol{\nabla}_x \bar{\phi} + \boldsymbol{\nabla}_y \phi^{(1)}] + \delta^1[\boldsymbol{\nabla}_x \phi^{(1)} + \boldsymbol{\nabla}_y \phi^{(2)}] + O(\delta^2), \\ \Delta \phi^\delta &= \delta^{-2}[\Delta_y \bar{\phi}] + \delta^{-1}[2\boldsymbol{\nabla}_x \cdot \boldsymbol{\nabla}_y \bar{\phi} + \Delta_y \phi^{(1)}] + \delta^0[\Delta_x \bar{\phi} + 2\boldsymbol{\nabla}_x \cdot \boldsymbol{\nabla}_y \phi^{(1)} + \Delta_y \phi^{(2)}] + O(\delta). \end{aligned} \tag{A.5}$$

Inserting this into equation (2.5) and setting the coefficients associated with the various powers of δ to zero, yields a sequence of problems.

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

$$\partial_\tau \phi^{(1)} - \varepsilon \Delta_y \phi^{(1)} - \boldsymbol{u} \cdot \boldsymbol{\nabla}_y \phi^{(1)} = \boldsymbol{u} \cdot \boldsymbol{\nabla}_x \bar{\phi}, \tag{A.6}$$

$$\partial_\tau \phi^{(2)} - \boldsymbol{u} \cdot \boldsymbol{\nabla}_y \phi^{(2)} - \varepsilon \Delta_y \phi^{(2)} = -\partial_t \bar{\phi} + \boldsymbol{u} \cdot \boldsymbol{\nabla}_x \phi^{(1)} + \varepsilon[\Delta_x \bar{\phi} + 2\boldsymbol{\nabla}_x \cdot \boldsymbol{\nabla}_y \phi^{(1)}]. \tag{A.7}$$

By the linearity of equation (A.6), we may separate the fast and slow variables by writing [59]

$$\phi^{(1)}(t, \boldsymbol{x}, \tau, \boldsymbol{y}) = \boldsymbol{\chi}(\tau, \boldsymbol{y}) \cdot \boldsymbol{\nabla}_x \bar{\phi}(t, \boldsymbol{x}). \tag{A.8}$$

When the components χ_k, $k = 1, \ldots, d$, of $\boldsymbol{\chi}$ satisfy the "cell problem"

$$\partial_\tau \chi_k - \varepsilon \Delta_y \chi_k - \boldsymbol{u} \cdot \boldsymbol{\nabla}_y \chi_k = \boldsymbol{u} \cdot \boldsymbol{e}_k, \tag{A.9}$$

equation (A.6) is automatically satisfied [59]. Equation (A.9) along with (4.13) is equivalent to the cell problem (4.15), where the distinction of fast variables was dropped for notational simplicity. In order for $\phi^{(1)}(t, \boldsymbol{x}, \tau, \boldsymbol{y})$ in (A.8) to be periodic in $(\tau, \boldsymbol{y})$ for each fixed $(t, \boldsymbol{x})$, we must have that the functions $\chi_k(\tau, \boldsymbol{y})$, $k = 1, \ldots, d$, are periodic. This and the fundamental theorem of calculus implies that $\langle \boldsymbol{\nabla}_y \chi_k \rangle = 0$. Here, $\langle \cdot \rangle$ denotes space-time averaging with respect to the *fast variables*.

Due to the incompressibility of the velocity field $\boldsymbol{\nabla}_y \cdot \boldsymbol{u}(\tau, \boldsymbol{y}) = 0$ and the *a priori* fast variable periodicity of the functions $\phi^{(i)}$, $i = 1, 2$, the fundamental theorem of calculus and the divergence theorem shows that the average of the left-hand-sides of equations (A.6) and (A.7) are zero. For the equations to have solutions, the average of the right-hand-sides must also vanish. The resulting solvability conditions are $\langle \boldsymbol{u} \rangle = 0$ and the following equation which governs the large-scale (slow variable) dynamics

$$\partial_t \bar{\phi} = \varepsilon \Delta_x \bar{\phi} + \langle \boldsymbol{u} \cdot \boldsymbol{\nabla}_x \phi^{(1)} \rangle. \tag{A.10}$$

Here, we have used that $\bar{\phi}$ is a *constant* with respect to the fast variables and, by the divergence theorem and the fast variable periodicity of $\phi^{(1)}$, we have $\langle \boldsymbol{\nabla}_y \cdot \boldsymbol{\nabla}_x \phi^{(1)} \rangle = 0$. The convergence of ϕ^δ to $\bar{\phi}$ as $\delta \to 0$ is in L^2 [27],

$$\lim_{\delta\to 0}\left[\sup_{0\le t\le t_0}\int \left|\phi^\delta(t,\boldsymbol{x}) - \bar{\phi}(t,\boldsymbol{x})\right|^2 \mathrm{d}\boldsymbol{x}\right] = 0, \tag{A.11}$$

for all $t_0 < \infty$, where we have used the notation $\mathrm{d}\boldsymbol{x} = \mathrm{d}x_1 \cdots \mathrm{d}x_d$ for the product Lebesgue measure.

Inserting equation (A.8) into (A.10) yields equation (2.3) with the components $\mathsf{D}^*_{jk} = \mathsf{D}^*\boldsymbol{e}_j \cdot \boldsymbol{e}_k$ of the effective diffusivity tensor D^* given by

$$\mathsf{D}^*_{jk} = \varepsilon\delta_{jk} + \langle u_j \chi_k\rangle. \tag{A.12}$$

By inserting the representation for u_j in (A.9) into equation (A.12), the functional $\langle u_j\chi_k\rangle$ can be represented in terms of $\boldsymbol{\nabla}_y\chi_j$ and the *skew-symmetric* operator $\mathbf{S} = \mathsf{H} + (-\Delta_y)^{-1}\mathbf{T}$, where the inverse operation $(-\Delta_y)^{-1}$ is based on convolution with the Green's function for the Laplacian Δ_y, $\mathbf{T} = \partial_\tau \mathsf{I}$, and the I in this definition is to remind us that the derivative ∂_τ operates component-wise. Indeed, writing $\partial_\tau\chi_j = \boldsymbol{\nabla}_y \cdot (\Delta_y^{-1}\mathbf{T})\boldsymbol{\nabla}_y\chi_j$, $\Delta_y\chi_j = \boldsymbol{\nabla}_y \cdot \boldsymbol{\nabla}_y\chi_j$, and $\boldsymbol{u} = \boldsymbol{\nabla}_y \cdot \mathsf{H}$ in (4.13), we have

$$\begin{aligned}\langle u_j\chi_k\rangle &= \langle[\partial_\tau\chi_j - \varepsilon\Delta_y\chi_j - \boldsymbol{u}\cdot\boldsymbol{\nabla}_y\chi_j]\chi_k\rangle\\ &= \langle\boldsymbol{\nabla}_y\cdot[(\Delta_y^{-1}\mathbf{T} - \varepsilon\mathsf{I} - \mathsf{H})\boldsymbol{\nabla}_y\chi_j]\chi_k\rangle\\ &= \langle[(\mathsf{H} + (-\Delta_y)^{-1}\mathbf{T} + \varepsilon\mathsf{I})\boldsymbol{\nabla}_y\chi_j]\cdot\boldsymbol{\nabla}_y\chi_k\rangle\\ &= \langle\mathbf{S}\boldsymbol{\nabla}_y\chi_j\cdot\boldsymbol{\nabla}_y\chi_k\rangle + \varepsilon\langle\boldsymbol{\nabla}_y\chi_j\cdot\boldsymbol{\nabla}_y\chi_k\rangle,\end{aligned} \tag{A.13}$$

where we have used the periodicity of χ_k and H to obtain the third equality. Equations (A.12) and (4.17) are equivalent to equations (**??**) and (4.14), where the distinction of fast variables was dropped for notational simplicity.

The above analysis shows that the main part of the study of effective, diffusive transport enhanced by periodic, incompressible flows, is the study of equation (A.9), from which the effective diffusivity tensor D^* emerges. In Section 6, we use the analytical structure of the cell problem (A.9) to derive a resolvent representation for $\boldsymbol{\nabla}_y\chi_k$, involving an anti-symmetric integro-differential operator $\mathbf{A}$ which is related to $\mathbf{S} = \mathsf{H} - \boldsymbol{\Delta}^{-1}\partial_t\mathsf{I}$. In Section 7, we employ this representation for $\boldsymbol{\nabla}_y\chi_k$ and the spectral theorem, to provide integral representations for D^* and A^* involving a *spectral measure* associated with the operator $\mathbf{A}$ acting on a suitable Hilbert space.

A.3. Existence and Uniqueness. THIS SECTION IS UNDER CONSTRUCTION

Before we discuss how the Hilbert space framework presented above leads to an integral representation for D^*, we first discuss some key differences in the theory between the cases of steady and dynamic velocity fields $\boldsymbol{u}$. These differences are reflected in the measure underlying this integral representation for D^* and stem from the *unboundedness* of the operator ∂_t on the Hilbert space $\mathcal{H}_\mathcal{T}$ [77, 85]. For steady $\boldsymbol{u}$, in general, equation (5.11) reduces to (4.14) for diagonal components of the effective parameter. However, for dynamic $\boldsymbol{u}$, this is not true in general. The details are as follows. For dynamic $\boldsymbol{u}$, the operator $\boldsymbol{\sigma}$ in (5.10) can be written as $\boldsymbol{\sigma} = \varepsilon\mathsf{I} + \mathbf{S}$, where $\mathbf{S} = \mathsf{H} - \boldsymbol{\Delta}^{-1}\partial_t\mathsf{I}$ is skew-symmetric $\langle\mathbf{S}\boldsymbol{\psi},\boldsymbol{\varphi}\rangle = -\langle\boldsymbol{\psi},\mathbf{S}\boldsymbol{\varphi}\rangle$ for all $\boldsymbol{\psi},\boldsymbol{\varphi}\in\mathcal{F}$ such that $|\langle\partial_t\boldsymbol{\psi},\boldsymbol{\varphi}\rangle|, |\langle\boldsymbol{\psi},\partial_t\boldsymbol{\varphi}\rangle| < \infty$ (see Section A for details). This property of the operator $\mathbf{S}$ implies that

$$\langle\mathbf{S}\boldsymbol{\psi}\cdot\boldsymbol{\psi}\rangle = -\langle\mathbf{S}\boldsymbol{\psi}\cdot\boldsymbol{\psi}\rangle = 0, \qquad \mathbf{S} = \mathsf{H} - (\boldsymbol{\Delta}^{-1})\partial_t\mathsf{I}, \tag{A.14}$$

for all such $\boldsymbol{\psi}\in\mathcal{F}$. In this dynamic setting, equation (5.8) does not hold for every $\boldsymbol{\psi}\in\mathcal{F}$, as the unbounded operator ∂_t is defined only on a proper (dense) subset of the Hilbert space $\mathcal{H}_\mathcal{T}$ [77], and it may be that $|\langle\partial_t\boldsymbol{\psi},\boldsymbol{\psi}\rangle| = \infty$. In the case of a steady velocity field we have $\mathbf{S}\equiv\mathsf{H}$ and, by equation (6.3) and the Cauchy Schwartz inequality, $|\langle\mathbf{S}\boldsymbol{\psi},\boldsymbol{\psi}\rangle| \le \|\mathsf{H}\|\|\boldsymbol{\psi}\|^2 < \infty$ for all $\boldsymbol{\psi}\in\mathcal{F}$, so equation (5.8) holds for all $\boldsymbol{\psi}\in\mathcal{F}$.

Another immediate consequence of equation (5.8), for steady $\boldsymbol{u}$, is the coercivity of the bilinear functional $\Phi(\boldsymbol{\psi},\boldsymbol{\varphi}) = \langle\boldsymbol{\sigma}\boldsymbol{\psi}\cdot\boldsymbol{\varphi}\rangle$ for all $\varepsilon > 0$. By equation (6.3), this functional is also bounded in the case of steady $\boldsymbol{u}$ for all $\varepsilon < \infty$. Therefore, the Lax-Milgram theorem [61] provides the existence and uniqueness of a solution $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$ satisfying the cell problem (4.15), or equivalently equation (5.10), in this time-independent case. The details are as follows.

The distributional form of equation (4.15), written as $\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\boldsymbol{e}_k=0$, is given by $\langle\boldsymbol{\sigma}(\boldsymbol{\nabla}\chi_k+\boldsymbol{e}_k)\cdot\boldsymbol{\nabla}\varphi\rangle=0$, where φ is a compactly supported, infinitely differentiable function on $\mathcal{T}\otimes\mathcal{V}$, and we stress that $\boldsymbol{\nabla}\varphi$ is *curl-free*. Motivated by this, we consider the following variational problem: find $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$ such that

$$\langle\boldsymbol{\sigma}(\boldsymbol{\nabla}\chi_k+\boldsymbol{e}_k)\cdot\boldsymbol{\psi}\rangle=0,\ \text{for all}\ \boldsymbol{\psi}\in\mathcal{F}. \tag{A.15}$$

In order to directly apply the Lax-Milgram Theorem, we rewrite equation (A.15) as

$$\Phi(\boldsymbol{\nabla}\chi_k,\boldsymbol{\psi})=\langle\boldsymbol{\sigma}\boldsymbol{\nabla}\chi_k\cdot\boldsymbol{\psi}\rangle=-\langle\boldsymbol{\sigma}\boldsymbol{e}_k\cdot\boldsymbol{\psi}\rangle=f(\boldsymbol{\psi}). \tag{A.16}$$

By equation (5.8) Φ is coercive, i.e.

$$\Phi(\boldsymbol{\psi},\boldsymbol{\psi})=\langle[(\varepsilon\mathsf{I}+\mathbf{S})]\boldsymbol{\psi}\cdot\boldsymbol{\psi}\rangle=\varepsilon\|\boldsymbol{\psi}\|^2>0,\ \text{for all}\ \boldsymbol{\psi}\in\mathcal{F} \tag{A.17}$$

such that $\|\boldsymbol{\psi}\|\neq 0$ and $\varepsilon>0$, where $\|\cdot\|$ is the norm induced by the inner-product $\langle\cdot,\cdot\rangle$. Recall that $\mathbf{S}=\mathsf{H}$ in this time-independent case. This, equation (6.3), the triangle inequality, and the Cauchy-Schwartz inequality imply that Φ is also bounded for all $\varepsilon<\infty$

$$\Phi(\boldsymbol{\psi},\boldsymbol{\varphi})\leq(\varepsilon+\|H\|)\|\boldsymbol{\psi}\|\|\boldsymbol{\varphi}\|<\infty,\ \text{for all}\ \boldsymbol{\psi}\in\mathcal{F}. \tag{A.18}$$

For the same reasons, the linear functional $f(\boldsymbol{\psi})$ in (A.16) is bounded for all $\boldsymbol{\psi}\in\mathcal{F}$. Therefore, the Lax-Milgram theorem [61] provides the existence of a unique $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$ satisfying (4.15) in this time-independent case.

In the time-dependent case, equation (5.8) hence (A.17) does not hold for all $\boldsymbol{\psi}\in\mathcal{F}$. Moreover, the operator ∂_t hence $\boldsymbol{\sigma}$ is not bounded on $\mathcal{F}$ [77, 83], so (A.18) does not hold. Consequently, the Lax-Milgram theorem cannot be directly applied, and alternate techniques [33, 34] must be used to prove the existence and uniqueness of a solution $\boldsymbol{\nabla}\chi_k\in\mathcal{F}$ satisfying the cell problem (4.15). This discussion illustrates key differences in the analytic structure of the effective parameter problem for D^*, between the cases of steady and dynamic velocity fields $\boldsymbol{u}$, which stem from the unboundedness of the operator ∂_t on $\mathcal{H}_\mathcal{T}$, hence $\boldsymbol{\sigma}$ on $\mathcal{F}$. In Section 7, we will discuss other consequences of this boundedness/unboundedness property of the operator $\boldsymbol{\sigma}$, and demonstrate that it leads to significant differences in the spectral measure underlying an integral representation of D^*.

A.4. Discrete integral representations by eigenfunction expansion. The integral representations of Theorem 7.1 and Corollary 7.2 for S^*_{jk} and A^*_{jk}, displayed in equation (7.7), involve spectral measures $\mathrm{d}\mu_{jk}(\lambda)$, $j,k=1,\ldots,d$, which have discrete and continuous components [77, 85]. In this section, we review these properties of $\mathrm{d}\mu_{jk}(\lambda)$ and provide an explicit derivation of the discrete component of these integrals. The explicit representation of the underlying discrete measure will be used extensively in Section 8, which exploits Fourier methods to calculate S^*_{jk} and A^*_{jk} for a large class of velocity fields. This, in turn, provides numerical methods for the computation of S^*_{jk} and A^*_{jk} for such velocity fields, which will be exploited in Section 10.

We now summarize some general spectral properties of the maximal, anti-symmetric operators $\mathbf{A}$ and A on the function spaces $\mathcal{F}$ and $\mathscr{F}$ defined in equations (6.4) and (4.3), respectively, which are dense subsets of their associated Hilbert spaces $\mathcal{H}_W$ and $\mathscr{H}^1$,

$$\mathcal{H}_W=\{\boldsymbol{\psi}\in\mathcal{H}_\mathcal{T}\otimes\mathcal{H}_W\,|\,\langle\boldsymbol{\psi}\rangle=0\},\quad \mathscr{H}^1=\{f\in\mathscr{H}_\mathcal{T}\otimes\mathscr{H}^1_\mathcal{V}\,|\,\langle f\rangle=0\}. \tag{A.19}$$

See equations (4.10) and (4.1) for the notational definitions of equation (A.19). For simplicity, we focus on the opertor A and the Hilbert space $\mathscr{H}^1$, as the discussion regarding $\mathbf{A}$ and $\mathcal{H}_W$ is analogous.

Recall that the domain $D(A)$ of the maximal normal operator A comprises those and only those elements $f\in\mathscr{F}$ such that $\|Af\|_1^2=\int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}\|Q(\lambda)f\|_1^2<\infty$, where $Q(\lambda)$ is the projection valued operator corresponding to A [85]. The integration is over the spectrum $\Sigma(A)$ of A, which has continuous $\Sigma_{\rm cont}$ and discrete (pure-point) $\Sigma_{\rm pp}$ components, $\Sigma(A)=\Sigma_{\rm cont}(A)\cup\Sigma_{\rm pp}(A)$. We first focus on the discrete spectrum $\Sigma_{\rm pp}(A)$. The members $f\neq 0$ of $D(A)$ which satisfy $Af=\upsilon f$ with $\upsilon\in\Sigma_{\rm pp}(A)$ are called eigenfunctions and υ is the corresponding eigenvalue. The span of all eigenfunctions is a *countable* subspace of $D(A)$ [77, 85]. Accordingly, we will denote the eigenfunctions by φ_n, $n=1,2,\ldots$, with corresponding eigenvalues υ_n. Since

A is anti-symmetric, υ_n is purely imaginary [85, 42] and we write $\upsilon_n = \imath\lambda_n$, where $\lambda_n \in \mathbb{R}$. Moreover, eigenfunctions corresponding to distinct eigenvalues are orthogonal and can be normalized to be orthonormal [85], i.e. if $A\varphi_n = \upsilon_n\varphi_n$, $A\varphi_m = \upsilon_m\varphi_m$, and $\upsilon_n \neq \upsilon_m$, then

$$\langle\varphi_n, \varphi_m\rangle_1 = \langle\boldsymbol{\nabla}\varphi_n \cdot \boldsymbol{\nabla}\varphi_m\rangle = \delta_{nm}. \tag{A.20}$$

There may be more than one eigenfunction associated with a particular eigenvalue. However, they are linearly independent and, without loss of generality, may be taken to be orthonormal [85]. Consequently, associated with each eigenfunction φ_n is a closed linear manifold, which we denote by $\mathcal{M}(\varphi_n)$. When $m \neq n$, $\mathcal{M}(\varphi_m)$ and $\mathcal{M}(\varphi_n)$ are mutually orthogonal. Set $\mathcal{E} = \oplus_{n=1}^{\infty}\mathcal{M}(\varphi_n)$, $\mathcal{M} = \mathcal{E} \oplus \{0\}$, and let $\mathcal{N} = \mathcal{M}^{\perp}$ be the orthogonal complement of $\mathcal{M}$ in $\mathscr{H}^1$.

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

Theorem A.1 ([85] pages 189 and 247). *One of the three cases must occur:*

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

In each of the three cases, the closed linear manifolds $\mathcal{M}$ and $\mathcal{N}$ reduce A [85].

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

Theorem A.2. *The following are equivalent, necessary and sufficient conditions that an element $\varphi_n \in D(A)$ be an eigenfunction with eigenvalue $\upsilon_n = \imath\lambda_n$, $\upsilon_n \in \Sigma_{pp}$.*

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

An immediate corrolary of this theorem is the following. If φ_n is an eigenfunction associated with the eigenvalue $\upsilon_n = \imath\lambda_n$, then [85]

$$\|A\varphi_n\|_1^2 = \int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}\|Q(\lambda)\varphi_n\|_1^2 = \lambda_n^2, \qquad \langle A\varphi_n, h\rangle_1 = \int_{-\infty}^{\infty}\lambda\,\mathrm{d}\langle Q(\lambda)\varphi_n, h\rangle_1 = \lambda_n\langle\varphi_n, h\rangle_1, \tag{A.21}$$

for all $h \in D(A)$. Moreover, a necessary and sufficient condition that $f \neq 0$ be and element of $\mathcal{M}$ in cases (2) and (3) of Theorem A.1 is that

$$f = \sum_{n=1}^{\infty} a_n\varphi_n, \quad a_n = \langle f, \varphi_n\rangle_1, \quad \|f\|_1^2 = \sum_{n=1}^{\infty}|a_n|^2 \neq 0. \tag{A.22}$$

Furthermore, for such an element f we have

$$\|Q(\lambda)f\|_1^2 = \sum_{n:\,\lambda_n \leq \lambda}|a_n|^2, \quad A\varphi_n = \imath\lambda_n\varphi_n. \tag{A.23}$$

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

THEOREM A.3 ([85] page 250). *The orthonormal set $\{\varphi_m\}$ of Theorem A.1 can be replaced by an orthonormal set $\{\phi_m\}$ such that*

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

$$\varrho_{k+1}(\lambda) = \int_{-\infty}^{\lambda} F(\psi)\mathrm{d}\varrho_k(\psi), \qquad \varrho_k(\lambda) = \|Q(\lambda)\phi_k\|_1^2, \qquad F(\lambda) = \frac{\mathrm{d}\varrho_{k+1}}{\mathrm{d}\varrho_k}, \tag{A.24}$$

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

The following theorem [85] provides an explicit representation for the standard decomposition of the Stieltjes measure $\mathrm{d}\mu(\lambda)$ into its continuous and discrete components.

THEOREM A.4 ([85] page 189). *Let f be an arbitrary element of $D(A)$, and g and h be its (unique) projections on $\mathcal{M}$ and $\mathcal{N}$, respectively, then the equation*

$$\|Q(\lambda)f\|_1^2 = \|Q(\lambda)g\|_1^2 + \|Q(\lambda)h\|_1^2, \qquad \mathrm{d}\|Q(\lambda)f\|_1^2 = \mathrm{d}\|Q(\lambda)g\|_1^2 + \mathrm{d}\|Q(\lambda)h\|_1^2 \tag{A.25}$$

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. The function space $\mathcal{N}$ can be further decomposed [77] $\mathcal{N} = \mathcal{N}_{\rm ac} \otimes \mathcal{N}_{\rm sing}$, with $h = h_{\rm ac} + h_{\rm sing}$, to provide the standard [32] decomposition of the continuous measure $\mathrm{d}\|Q(\lambda)h\|_1^2$ into its components which are absolutely continuous and singular with respect to the Lebesgue measure, respectively,

$$\mathrm{d}\|Q(\lambda)h\|_1^2 = \mathrm{d}\|Q(\lambda)h_{\rm ac}\|_1^2 + \mathrm{d}\|Q(\lambda)h_{\rm sing}\|_1^2. \tag{A.26}$$

However, the sets $\mathcal{N}_{\rm ac}$ and $\mathcal{N}_{\rm sing}$ need not be disjoint [77].

We now use the mathematical framework summarized above to provide explicit formulas for the discrete component of the integral representations for S^*_{jk} and A^*_{jk}, displayed in equation (7.7). For simplicity, we focus on the formulation of the effective parameter problem described by Corollary 7.2, as that of Theorem 7.1 is analogous. Recall the cell problem of equations (4.7) and (A.9), written as

$$(\varepsilon + A)\chi_j = g_j, \quad g_j = (-\Delta)^{-1}u_j, \tag{A.27}$$

where A is defined in equation (4.4) and u_j, $j = 1,\dots,d$, is the $j^{\rm th}$ component of the velocity field $\boldsymbol{u}$. Since $\chi_j, g_j \in \mathscr{F} \subset \mathscr{H}^1$, by the formula $\mathscr{H}^1 = \mathcal{M} \oplus \mathcal{N}$ of Theorem A.1 and equation (A.22), they have the following representations

$$\chi_j = \sum_n \langle\varphi_n, \chi_j\rangle_1\, \varphi_n + \chi_j^{\perp}, \qquad g_j = \sum_n \langle\varphi_n, g_j\rangle_1\, \varphi_n + g_j^{\perp}, \tag{A.28}$$

where $\varphi_n \in \mathcal{M}$ and $\chi_j^{\perp}, g_j^{\perp} \in \mathcal{N}$. Inserting (A.28) into the cell problem (A.27) and using $A\varphi_n = \imath\lambda_n\varphi_n$ yields

$$\sum_n [(\varepsilon + \imath\lambda_n)\langle\varphi_n, \chi_j\rangle_1 - \langle\varphi_n, g_j\rangle_1]\varphi_n + (\varepsilon + A)\chi_j^{\perp} - g_j^{\perp} = 0. \tag{A.29}$$

By the orthonormality of the set $\{\varphi_n\}$, the mutual orthogonality of the manifolds $\mathcal{M}$ and $\mathcal{N}$, and since $\langle A\chi_j^{\perp}, \varphi_n\rangle_1 = -\langle\chi_j^{\perp}, A\varphi_n\rangle_1 = -\imath\lambda_n\langle\chi_j^{\perp}, \varphi_n\rangle_1 = 0$, taking the inner-product of both sides of (A.29) with φ_n yields

$$\langle\varphi_n, \chi_j\rangle_1 = \frac{\langle\varphi_n, g_j\rangle_1}{(\varepsilon + \imath\lambda_n)}, \quad 0 < \varepsilon < \infty. \tag{A.30}$$

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 (4.4). From equations (A.28) and (A.30), the orthonormality of the set $\{\varphi_n\}$, and the mutual orthogonality of $\mathcal{M}$ and $\mathcal{N}$, we have

$$\text{(A.31)}\qquad \langle\chi_j,\chi_k\rangle_1-\langle\chi_j^\perp,\chi_k^\perp\rangle_1=\sum_n\overline{\langle\varphi_n,\chi_j\rangle}_1\langle\varphi_n,\chi_k\rangle_1=\sum_n\frac{\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1}{\varepsilon^2+\lambda_n^2}$$
$$\langle A\chi_j,\chi_k\rangle_1-\langle A\chi_j^\perp,\chi_k^\perp\rangle_1=\sum_n-\imath\lambda_n\,\overline{\langle\varphi_n,\chi_j\rangle}_1\langle\varphi_n,\chi_k\rangle_1=\sum_n\frac{-\imath\lambda_n\,\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1}{\varepsilon^2+\lambda_n^2}\,.$$

The right hand sides of the formulas in equation (A.31) 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 $\mathrm{d}\langle Q(\lambda)g_j^\perp,g_k^\perp\rangle_1$, and provides the standard decomposition of the *spectral measure* into its discrete and continuous components, in the general setting [85].

A direct correspondence can be made between the integrals in equations (A.31) and (7.7) with use of Dirac's bra-ket notation as follows. Writing $\mu_{jk}(\lambda)=\langle Q(\lambda)g_j,g_k\rangle_1=\langle g_j,Q(\lambda)g_k\rangle_1=\langle g_j|Q(\lambda)|g_k\rangle$ and recalling the property $\overline{\langle\varphi_n,g_j\rangle}_1=\langle g_j,\varphi_n\rangle_1$ and that g_j is real-valued, suggests the notation

$$\text{(A.32)}\qquad \overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1=\langle g_j|\,|\varphi_n\rangle\overline{\langle\varphi_n|}\,|g_j\rangle=\langle g_j|Q_n|g_k\rangle,$$

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

$$\text{(A.33)}\qquad \mathrm{d}\mu_{jk}(\lambda)=\langle g_j|Q(\lambda)|g_k\rangle\,\delta_{\lambda_n}(\mathrm{d}\lambda),\qquad Q(\lambda)=\sum_{n:\,\lambda_n\le\lambda}Q_n,\quad Q_n=|\varphi_n\rangle\overline{\langle\varphi_n|},\quad \lambda\in\Sigma_{\mathrm{pp}}(A),$$

where $\delta_{\lambda_n}(\mathrm{d}\lambda)$ is the delta measure concentrated at λ_n. Moreover, exactly as in equations (7.11) and (7.13), we may use the fact that the function g_j and molecular diffusivity ε are real-valued, to re-express the integrals in (A.31), involving the *complex measure* $\mathrm{d}\mu_{jk}(\lambda)$, in terms of the *signed measures* $\mathrm{dRe}\,\mu_{jk}(\lambda):=(\mathrm{d}\mu_{jk}(\lambda)+\mathrm{d}\mu_{kj}(\lambda))/2$ and $\mathrm{dIm}\,\mu_{jk}(\lambda):=(\mathrm{d}\mu_{jk}(\lambda)-\mathrm{d}\mu_{kj}(\lambda))/(2\imath)$, where

$$\text{(A.34)}\qquad \mathrm{dRe}\,\mu_{jk}(\lambda)=\mathrm{Re}\langle g_j|Q(\lambda)|g_k\rangle\;\delta_{\lambda_n}(\mathrm{d}\lambda),\qquad \mathrm{Re}\langle g_j|Q(\lambda)|g_k\rangle=\sum_{n:\,\lambda_n\le\lambda}\mathrm{Re}[\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1]$$
$$\mathrm{dIm}\,\mu_{jk}(\lambda)=\mathrm{Im}\langle g_j|Q(\lambda)|g_k\rangle\;\delta_{\lambda_n}(\mathrm{d}\lambda),\qquad \mathrm{Im}\langle g_j|Q(\lambda)|g_k\rangle=\sum_{n:\,\lambda_n\le\lambda}\mathrm{Im}[\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1].$$

A usefull property of the inner-product $\langle\varphi_n,g_k\rangle_1$ and the form of $g_j=(-\Delta)^{-1}u_j$ is that $\langle\varphi_n,g_j\rangle_1=\langle\varphi_n,u_j\rangle_2$. More specifically, since $u_j(t,\cdot)\in\mathscr{H}^1(\mathcal{V})\subset L^2(\mathcal{V})$ we have [83]

$$\text{(A.35)}\qquad \langle\varphi_n,g_j\rangle_1=\langle\boldsymbol{\nabla}\varphi_n\cdot\boldsymbol{\nabla}(-\Delta)^{-1}u_j\rangle=\langle\varphi_n,(-\Delta)(-\Delta)^{-1}u_j\rangle_2=\langle\varphi_n,u_j\rangle_2,$$

where $\langle\cdot,\cdot\rangle_2$ denotes the $L^2(\mathcal{T}\times\mathcal{V})$ inner-product. This property will be used in Section 8 to calculate S^*_{jk} and A^*_{jk} for a large class of velocity fields.

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