SPECTRAL THEORY OF ADVECTIVE DIFFUSION BY DYNAMIC AND STEADY PERIODIC FLOWS

N. B. MURPHY*, J. XIN†, J. ZHU*, AND E. CHERKAEV‡

Department of Mathematics, University of California at Irvine

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

1. Introduction

The long time, large scale behavior of a diffusing particle or tracer being advected by an incompressible velocity field is equivalent to an enhanced diffusive process [35] with an effective diffusivity tensor $\mathcal{K}^*$. Determining the effective transport properties of advection enhanced diffusion is a challenging problem with theoretical and practical importance in many fields of science and engineering, ranging from turbulent combustion to mass, heat, and salt transport in geophysical flows [24]. A broad range of mathematical techniques have been developed that reduce the analysis of complex fluid flows, with rapidly varying structures in space and time, to solving averaged or *homogenized* equations that do not have rapidly varying data, and involve an effective parameter.

Homogenization of the advection-diffusion equation for thermal transport by random, time-independent fluid velocity fields was treated in [21]. This reduced the analysis of turbulent diffusion to solving a diffusion equation involving a homogenized temperature and a (constant) effective diffusivity tensor $\mathcal{K}^*$. An important consequence of this analysis is that $\mathcal{K}^*$ is given in terms of a *curl-free* stationary stochastic process which satisfies a steady state diffusion equation, involving a skew-symmetric random matrix $\mathbf{H}$ [2, 1]. By adapting the analytic continuation method (ACM) of homogenization theory for composites [15], it was shown that the result in [21] leads to an integral representation for the symmetric part $\boldsymbol{\kappa}^*$ of $\mathcal{K}^*$, involving a spectral measure of a self-adjoint random operator [2, 1]. This integral representation of $\boldsymbol{\kappa}^*$ was generalized to the time-dependent case in [3, 7]. Remarkably, this method has also been extended to flows with incompressible *nonzero* effective drift [29], flows where particles diffuse according to linear collisions [30], and solute transport in porous media [6]. All these approaches yield integral representations of the symmetric and, when appropriate, the anti-symmetric part $\boldsymbol{\alpha}^*$ of $\mathcal{K}^*$.

Homogenization of the advection-diffusion equation for periodic or cellular, incompressible flow fields was treated in [9, 10]. As in the case of random flows, the effective diffusivity tensor $\mathcal{K}^*$ is given in terms of a *curl-free* vector field, which satisfies a diffusion equation involving a skew-symmetric matrix $\mathbf{H}$. Here, we demonstrate that the ACM can be adapted to this periodic setting to provide integral representations for both the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of $\mathcal{K}^*$, for both cases of steady and time-dependent flows. These integral representations involve a self-adjoint or normal linear operator and the (non-dimensional) molecular diffusivity ε. In the case of steady fluid velocity fields, the spectral measure is associated with a Hermitian Hilbert-Schmidt integral operator involving the Green's function of the Laplacian on a rectangle. While in the case of dynamic flows, the spectral measure is associated with a Hermitian operator which is the sum of that for steady flows and an unbounded integro-differential operator.

We utilize the analytic structure of the integral representation for $\boldsymbol{\mathcal{K}}^*$ to obtain its asymptotic behavior for model flows, as the molecular diffusivity ε tends to zero. This is the high Péclet number regime that is important for the understanding of transport processes in real fluid flows, where the molecular diffusivity is often quite small in comparison. In particular, necessary and sufficient conditions for steady periodic flow fields $\kappa^* \sim \epsilon^{1/2}$, generically, for steady flows and $\kappa^* \sim O(1)$ for "chaotic" time-dependent flows. To make this manuscript more self contained, we have include an appendix in Section A-1 which contains many of the technical details underlying this work. In Section 2, we formulate the effective parameter problem for enhanced diffusive transport by advective, periodic flows, which leads to a functional representation of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$. We provide integral representations for the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of $\boldsymbol{\mathcal{K}}^*$, which hold for both steady and dynamic flows. The effective parameter problem [21, 9, 7] for such transport processes is reviewed in Section 2, and parallels existing between this problem of homogenization theory [4] and the ACM for representing transport in composites [15] are put into correspondence. In particular, an abstract Hilbert space framework is provided in Section 3 which places these different effective parameter problems on common mathematical footing. Within this Hilbert space setting, we derive in Section 4 integral representations for $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$, involving the molecular diffusivity ε and a *spectral measure* of a self-adjoint (or equivalently a maximal normal) linear operator. These integral representations are employed in Section 6 to obtain the asymptotic behavior of the components of $\boldsymbol{\mathcal{K}}^*$ in the scaling regime, where $\varepsilon \ll 1$. FINISH THIS PARAGRAPH WHEN WE HAVE CONCRETE RESULTS.

2. Effective transport by advective-diffusion

In this section, we review the effective parameter problem for advection enhanced diffusion. For completeness and to streamline the presentation of this theory, many of the mathematical details are given in Section A-1.2 of the appendix. Consider the advection enhanced diffusive transport of a passive tracer $\phi(t,\vec{x}\,)$, $t>0$, $\vec{x}\in\mathbb{R}^d$, as described by the advection-diffusion equation

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

with initial density $\phi_0(\vec{x})$ given. Here, ∂_t denotes partial differentiation with respect to time t, $\Delta = \vec{\nabla}\cdot\vec{\nabla} = \nabla^2$ is the Laplacian, and $\kappa_0 > 0$ is the molecular diffusivity. The fluid velocity field $\vec{v} = \vec{v}(t,\vec{x})$ in (1) is assumed to be periodic, incompressible, and mean-zero,

$$\vec{\nabla}\cdot\vec{v} = 0, \quad \langle\vec{v}\,\rangle = 0, \tag{2}$$

where we denote by 0 the null element of all linear spaces in question. Consider the bounded sets $\mathcal{T}\subset\mathbb{R}$ and $\mathcal{V}\subset\mathbb{R}^d$, with $t\in\mathcal{T}$ and $\vec{x}\in\mathcal{V}$, which define the space-time period cell ($(d+1)$–torus) $\mathcal{T}\otimes\mathcal{V}$. In equation (2), we denote by $\langle\cdot\rangle$ spatial averaging over $\mathcal{V}$ in the case of a time-independent velocity field, $\vec{v} = \vec{v}(\vec{x})$, and when the velocity field is time-dependent, $\vec{v} = \vec{v}(t,\vec{x})$, $\langle\cdot\rangle$ denotes space-time averaging over $\mathcal{T}\otimes\mathcal{V}$. In the time-dependent case, we stress that $\langle\vec{v}\,\rangle = 0$ in (2) means that $\langle\vec{v}(t,\cdot)\rangle = 0$ *and* $\langle\vec{v}(\cdot,\vec{x})\rangle = 0$ for each $t\in\mathcal{T}$ and $\vec{x}\in\mathcal{V}$ fixed, respectively.

We non-dimensionalize equation (1) as follows. Let ℓ and $\tilde{t}$ be typical length and time scales associated with the problem of interest. Mapping to the non-dimensional variables $t\mapsto t/\tilde{t}$ and $x_j\mapsto x_j/\ell$, one finds that ϕ satisfies the advection-diffusion equation in (1) with a non-dimensional molecular diffusivity $\varepsilon = \tilde{t}\kappa_0/\ell^2$ and velocity field $\vec{u} = \tilde{t}\,\vec{v}/\ell$, where x_j is the j^{th} component of the vector $\vec{x}$.

For d-dimensional, mean-zero, incompressible flows $\vec{u}$, there is a real (non-dimensional) skew-symmetric matrix $\mathbf{H}(t,\vec{x})$ such that (see Section A-1.1 for details)

$$\vec{u} = \vec{\nabla}\cdot\mathbf{H}, \qquad \mathbf{H}^T = -\mathbf{H}, \tag{3}$$

where $\mathbf{H}^T$ denotes transposition of the matrix $\mathbf{H}$. Using this representation of the velocity field $\vec{u}$, which also satisfies (2), equation (1) can be written as a diffusion equation,

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

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

$$\kappa_{jk} = \varepsilon\delta_{jk} + H_{jk}, \quad j,k = 1,\cdots,d. \tag{5}$$

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

We are interested in the dynamics of ϕ in (4) for *large* length and time scales, and when the initial density ϕ_0 is slowly varying relative to the velocity field $\vec{u}$. Anticipating that ϕ will have diffusive dynamics, we re-scale space and time by $\vec{x}\mapsto\vec{x}/\delta$ and $t\mapsto t/\delta^2$, respectively. For periodic diffusivity coefficients in (4) which are uniformly elliptic but not necessarily symmetric, it can be shown [9] that, as $\delta\to 0$, the associated solution $\phi^\delta(t,\vec{x})$ of (4) converges to $\bar{\phi}(t,\vec{x})$, which satisfies the following diffusion equation involving a (constant) effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$

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

The components $\mathcal{K}^*_{jk} = \boldsymbol{\mathcal{K}}^*\vec{e}_j\cdot\vec{e}_k$ of the effective tensor $\boldsymbol{\mathcal{K}}^*$ are given by $\mathcal{K}^*_{jk} = \varepsilon\delta_{jk} + \langle u_j\chi_k\rangle$. For each standard basis vector $\vec{e}_k$, $k = 1,\ldots,d$, the function $\chi_k = \chi_k(t,\vec{x}\,;\vec{e}_k)$ satisfies [9] the cell problem

$$\partial_t\chi_k = \vec{\nabla}\cdot\boldsymbol{\kappa}(\vec{\nabla}\chi_k + \vec{e}_k\,), \quad \langle\vec{\nabla}\chi_k\rangle = 0. \tag{7}$$

Equation (7) also holds [9] when the velocity field is time-independent $\vec{u} = \vec{u}(\vec{x})$. However in this case, χ_k is also time-independent and $\partial_t\chi_k = 0$. The symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ are defined by

$$\boldsymbol{\mathcal{K}}^* = \boldsymbol{\kappa}^* + \boldsymbol{\alpha}^*, \qquad \boldsymbol{\kappa}^* = \frac{1}{2}\left(\boldsymbol{\mathcal{K}}^* + [\boldsymbol{\mathcal{K}}^*]^T\right), \quad \boldsymbol{\alpha}^* = \frac{1}{2}\left(\boldsymbol{\mathcal{K}}^* - [\boldsymbol{\mathcal{K}}^*]^T\right). \tag{8}$$

The components κ^*_{jk} and α^*_{jk}, $j,k = 1,\ldots,d$, of $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ can be written in terms of the following functionals involving the *real-valued* vector field $\vec{\nabla}\chi_k$

$$\kappa^*_{jk} = \varepsilon(\delta_{jk} + \langle\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle), \qquad \alpha^*_{jk} = \langle\mathbf{S}\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle, \qquad \mathbf{S} = \mathbf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}, \quad \mathbf{T} = \partial_t\mathbf{I}, \tag{9}$$

where $\vec{\xi}\cdot\vec{\zeta} = \vec{\xi}^\dagger\vec{\zeta}$ 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 $\mathcal{V}$ [33].

Due to the fact that the vector field $\vec{\nabla}\chi_j$ is *real-valued*, we have that $\langle\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle = \langle\vec{\nabla}\chi_k\cdot\vec{\nabla}\chi_j\rangle$. From equation (9) this clearly implies that the tensor $\boldsymbol{\kappa}^*$ is symmetric, $\kappa^*_{jk} = \kappa^*_{kj}$. Moreover, equation (9) demonstrates that the effective transport of the tracer ϕ in the principle directions $\vec{e}_k$, $k = 1,\ldots,d$, is always *enhanced* by the presence of an incompressible velocity field, $\mathcal{K}^*_{kk} = \kappa^*_{kk}\geq\varepsilon$. The equality $\mathcal{K}^*_{kk} = \kappa^*_{kk}$ follows from the skew-symmetry of $\boldsymbol{\alpha}^*$, so that $\alpha^*_{kj} = -\alpha^*_{jk}$ and $\alpha^*_{kk} = 0$. This, in turn, follows from the skew-symmetry of the operator $\mathbf{S}$ (see Section A-1.3), $\alpha^*_{jk} = \langle\mathbf{S}\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle = -\langle\mathbf{S}\vec{\nabla}\chi_k\cdot\vec{\nabla}\chi_j\rangle = -\alpha^*_{kj}$ and

$$\alpha^*_{kk} = \langle\mathbf{S}\vec{\nabla}\chi_k\cdot\vec{\nabla}\chi_k\rangle = -\langle\mathbf{S}\vec{\nabla}\chi_k\cdot\vec{\nabla}\chi_k\rangle = 0. \tag{10}$$

In Section 3 we discuss the properties of the linear operator $\mathbf{S}$ and the vector field $\vec{\nabla}\chi_j$ in more detail.

We now recast equations (7) and (9) 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 ACM for characterizing effective transport in composite media [15, 23]. 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 [15, 25, 23]. Here we establish a correspondence between this effective parameter problem and that for enhanced diffusive transport by advective velocity fields. In Section 3, we formulate the Hilbert space framework associated with advective diffusion, and employ it to obtain a resolvent representation of the vector field $\vec{\nabla}\chi_k$ in (7). In Section 4 we utilize this mathematical framework to obtain integral representations for $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$, involving a spectral measure which depends only on the fluid velocity field $\vec{u}$.

Toward this goal, we recast the first formula in equation (7) in a more suggestive, divergence form. Using the notation from equation (9) we write

$$\vec{\nabla}(\Delta^{-1})\partial_t = \boldsymbol{\Delta}^{-1}\mathbf{T}\vec{\nabla}, \tag{11}$$

so that [9] $\partial_t\chi_k = \Delta\Delta^{-1}\partial_t\chi_k = \vec{\nabla}\cdot(\boldsymbol{\Delta}^{-1}\mathbf{T})\vec{\nabla}\chi_k$. Define the vector field $\vec{E}_k = \vec{\nabla}\chi_k + \vec{e}_k$ and the operator $\boldsymbol{\sigma} = \boldsymbol{\kappa} - (\boldsymbol{\Delta}^{-1})\mathbf{T} = \varepsilon\mathbf{I} + \mathbf{S}$, where $\boldsymbol{\sigma} = \boldsymbol{\kappa} = \varepsilon\mathbf{I} + \mathbf{H}$ in the case of steady fluid velocity fields. With these definitions, equation (7) may be written as $\vec{\nabla}\cdot\boldsymbol{\sigma}\vec{E}_k = 0$, $\langle\vec{E}_k\rangle = \vec{e}_k$, which is equivalent to

$$\vec{\nabla}\cdot\vec{J}_k = 0, \quad \vec{\nabla}\times\vec{E}_k = 0, \quad \vec{J}_k = \boldsymbol{\sigma}\vec{E}_k, \quad \langle\vec{E}_k\rangle = \vec{e}_k, \qquad \boldsymbol{\sigma} = \varepsilon\mathbf{I} + \mathbf{S}. \tag{12}$$

The formulas in (12) are precisely the electrostatic version of Maxwell's equations for a conductive medium [15], where $\vec{E}_k$ and $\vec{J}_k$ are the local electric field and current density, respectively, and $\boldsymbol{\sigma}$ is the local conductivity tensor of the medium. In the ACM for composites, the effective conductivity tensor $\boldsymbol{\sigma}^*$ is defined as

$$\langle\vec{J}_k\rangle = \boldsymbol{\sigma}^*\langle\vec{E}_k\rangle. \tag{13}$$

The linear constitutive relation $\vec{J}_k = \boldsymbol{\sigma}\vec{E}_k$ in (12) relates the local intensity and flux, while that in (13) relates the mean intensity and flux. Due to the skew-symmetry of $\mathbf{S}$, the intensity-flux relationship in (12) is similar to that of a Hall medium [18].

For the (constant) tensors $\boldsymbol{\mathcal{K}}^*$ and $\boldsymbol{\sigma}^*$ to be meaningful, the averages which define these effective quantities in (9) and (13) must be well defined and finite. For example, in order for the diagonal components $\mathcal{K}^*_{kk}$, $k = 1,\ldots,d$, of $\boldsymbol{\mathcal{K}}^*$ to be well defined and finite, the vector field $\vec{\nabla}\chi_k$ must be Lebesgue measurable and square integrable on $\mathcal{T}\times\mathcal{V}$. Moreover, for the components α^*_{jk}, $j \neq k = 1,\ldots,d$, of $\boldsymbol{\alpha}^*$ to be well defined and finite, we must also have that the operator $\mathbf{S}$ is bounded in some sense so that $\mathbf{S}\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k$ is Lebesgue integrable on $\mathcal{T}\times\mathcal{V}$. In other words, we must define the vector field $\vec{\nabla}\chi_j$ as a member of a suitable space of functions so that the components of the tensors $\boldsymbol{\mathcal{K}}^*$ and $\boldsymbol{\sigma}^*$ are well defined and have finite values. In Section 3 we discuss these important details at length and prove the following theorem.

Theorem 2.1. *Let the components $\mathcal{K}^*_{jk}$ and σ^*_{jk}, $j,k = 1,\ldots,d$, of the effective tensors $\boldsymbol{\mathcal{K}}^*$ and $\boldsymbol{\sigma}^*$ be defined as in equations* (7)–(9) *and* (12)–(13)*, respectively. Then there exists a function space $\mathscr{F}$ on which $\boldsymbol{\sigma} = \varepsilon\mathbf{I} + \mathbf{S}$ is a bounded linear operator for all $0 < \varepsilon < \infty$ and, for $\vec{\nabla}\chi_j \in \mathscr{F}$, $\mathcal{K}^*_{jk}$ and σ^*_{jk} are well defined and finite. Moreover, these effective tensors are equivalent up to transposition,*

$$\boldsymbol{\sigma}^* = [\boldsymbol{\mathcal{K}}^*]^T. \tag{14}$$

In particular, the symmetric part $\boldsymbol{\kappa}^*$ of $\boldsymbol{\mathcal{K}}^*$ is equal to that of $\boldsymbol{\sigma}^*$ and the anti-symmetric part $\boldsymbol{\alpha}^*$ of $\boldsymbol{\mathcal{K}}^*$ is equal to the negative of that of $\boldsymbol{\sigma}^*$.

Theorem 2.1 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 $\vec{u}$. The validity of Theorem 2.1 follows by adapting the Hilbert space formulation of the ACM to treat the effective transport properties of advective diffusion, which is the topic of Section 3. This Hilbert space formulation of the effective parameter problem also leads to integral representations for $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$, which is the topic of Section 4.

3. Hilbert space and resolvent representation

In this section we explore the mathematical properties of the skew-symmetric operator $\mathbf{S}$ introduced in equation (9) and construct a function space $\mathscr{F}$ such that for $\vec{\nabla}\chi_k \in \mathscr{F}$ equation (14) 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 (7) to obtain a resolvent representation of the vector field $\vec{\nabla}\chi_k$, 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 4 integral representations for the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$, involving a *spectral measure* associated with $\mathbf{A}$.

Consider the Hilbert spaces $L^2_d(\mathcal{T}) = \otimes_{n=1}^d L^2(\mathcal{T})$ and $L^2_d(\mathcal{V}) = \otimes_{n=1}^d L^2(\mathcal{V})$ (over the complex field $\mathbb{C}$) of Lebesgue measurable, square integrable, vector-valued functions [12], where $\mathcal{T} \subset \mathbb{R}$ and $\mathcal{V} \subset \mathbb{R}^d$. Now consider the associated Hilbert spaces $\mathscr{H}_\mathcal{T} \subset L^2_d(\mathcal{T})$ and $\mathscr{H}_\mathcal{V} \subset L^2_d(\mathcal{V})$ 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 $\mathscr{H}_{\mathcal{T}\mathcal{V}}$,

$$\mathscr{H}_{\mathcal{T}\mathcal{V}} = \mathscr{H}_\mathcal{T} \otimes \mathscr{H}_\mathcal{V}, \quad \mathscr{H}_\mathcal{T} = \{\vec{\xi} \in L^2_d(\mathcal{T}) \mid \vec{\xi}(0) = \vec{\xi}(T)\}, \quad \mathscr{H}_\mathcal{V} = \{\vec{\xi} \in L^2_d(\mathcal{V}) \mid \vec{\xi}(0) = \vec{\xi}(\vec{V})\}, \tag{15}$$

where we have defined $\vec{V} = (V_1, \ldots, V_d)$. 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 $\langle \vec{\xi}, \vec{\zeta} \rangle = \langle \overline{\vec{\xi}} \cdot \vec{\zeta} \rangle$ with $\langle \vec{\xi}, \vec{\zeta} \rangle = \overline{\langle \vec{\zeta}, \vec{\xi} \rangle}$, where $\bar{a}$ denotes complex conjugation for $a \in \mathbb{C}$ and $(\overline{\vec{\xi}})_j = \overline{\xi_j}$, $j = 1, \ldots, d$. By the Helmholtz theorem [20, 5], the Hilbert space $\mathscr{H}_\mathcal{V}$ in (15) can be decomposed into mutually orthogonal subspaces of curl-free $\mathscr{H}_\times$, divergence-free $\mathscr{H}_\bullet$, and constant $\mathscr{H}_0$ vector fields, with associated orthogonal projectors $\boldsymbol{\Gamma}_\times$, $\boldsymbol{\Gamma}_\bullet$, and $\boldsymbol{\Gamma}_0$, respectively, [9, 23]

$$\begin{gathered}\mathscr{H}_\mathcal{V} = \mathscr{H}_\times \oplus \mathscr{H}_\bullet \oplus \mathscr{H}_0, \qquad \mathbf{I} = \boldsymbol{\Gamma}_\times + \boldsymbol{\Gamma}_\bullet + \boldsymbol{\Gamma}_0, \\ \boldsymbol{\Gamma}_\times = \vec{\nabla}(\Delta^{-1})\vec{\nabla}\cdot, \quad \boldsymbol{\Gamma}_\bullet = -\vec{\nabla} \times (\boldsymbol{\Delta}^{-1})\vec{\nabla}\times, \quad \boldsymbol{\Gamma}_0 = \langle \cdot \rangle, \\ \mathscr{H}_\times = \{\vec{\xi} \mid \vec{\nabla} \times \vec{\xi} = 0 \text{ weakly}\}, \quad \mathscr{H}_\bullet = \{\vec{\xi} \mid \vec{\nabla} \cdot \vec{\xi} = 0 \text{ weakly}\}, \quad \mathscr{H}_0 = \{\vec{\xi} \mid \vec{\xi} = \langle \vec{\xi} \rangle\}.\end{gathered} \tag{16}$$

We are primarily concerned with fluid velocity fields $\vec{u}$ such that $0 < \mathcal{K}^*_{kk} < \infty$ for all $0 < \varepsilon < \infty$. Consequently, in view of equation (9), we require that the (weakly) curl-free vector field $\vec{\nabla}\chi_k$ satisfies $\vec{\nabla}\chi_k \in \mathscr{H}_\mathcal{T} \otimes \mathscr{H}_\times \subset \mathscr{H}_{\mathcal{T}\mathcal{V}}$, so that it is bounded in the norm $\|\cdot\|$ induced by the $\mathscr{H}_{\mathcal{T}\mathcal{V}}$-inner-product [12], $\|\vec{\nabla}\chi_k\| < \infty$. Defining the (weakly) divergence-free vector field $\vec{J}_k = \boldsymbol{\sigma}\vec{E}_k$ in (12) as a member of a subset of $\mathscr{H}_{\mathcal{T}\mathcal{V}}$ is technically difficult, due to the *unboundedness* of the linear operator $\boldsymbol{\sigma} = \boldsymbol{\kappa} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ 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 [33] on the Hilbert space $L^2(\mathcal{V})$. Hence $(\boldsymbol{\Delta}^{-1})$ is a compact operator on the Hilbert space $\mathscr{H}_\mathcal{V}$, and is consequently bounded in the operator norm $\|\cdot\|$ induced by the $\mathscr{H}_{\mathcal{T}\mathcal{V}}$-inner-product [31, 34, 33], when considered as an operator on $\mathscr{H}_{\mathcal{T}\mathcal{V}}$. We have already assumed for the convergence $\phi^\delta \to \bar{\phi}$, as $\delta \to 0$, that the flow matrix $\mathbf{H}(t,\vec{x})$ is periodic on $\mathcal{T}\times\mathcal{V}$. We will also assume that it is (component-wise) mean-zero and bounded in operator norm, and that its component-wise time derivative $\mathbf{TH}$ is also bounded on $\mathscr{H}_{\mathcal{T}\mathcal{V}}$

$$\langle \mathbf{H}\rangle = 0, \quad \|\mathbf{H}\| < \infty, \quad \|\mathbf{TH}\| < \infty. \tag{17}$$

This implies that $\boldsymbol{\kappa} = \varepsilon\mathbf{I} + \mathbf{H}$ is also bounded for all $0 < \varepsilon < \infty$. Consequently, in the case of a time-independent velocity field $\vec{u}$, where $\boldsymbol{\sigma} = \boldsymbol{\kappa}$, the linear operator $\boldsymbol{\sigma}$ is bounded. This and $\|\vec{\nabla}\chi_k\| < \infty$ implies that $\vec{J}_k \in \mathscr{H}_\bullet$. Therefore, in the case of a time-dependent velocity field, under the assumptions of (17), the unboundedness of $\boldsymbol{\sigma} = \boldsymbol{\kappa} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ on $\mathscr{H}_{\mathcal{T}\mathcal{V}}$ is due to the unboundedness of $\mathbf{T}$ on $\mathscr{H}_{\mathcal{T}}$.

The unboundedness of $\mathbf{T}$ on $\mathscr{H}_{\mathcal{T}}$ can be understood by considering the orthonormal set of functions $\{\vec{\psi}_n\} \subset \mathscr{H}_{\mathcal{T}}$ with components $(\vec{\psi}_n)_j$, $j = 1,\ldots,d$, defined by

$$(\vec{\psi}_n)_j(t) = \beta \sin((n+j)\pi t/T), \quad \beta = \sqrt{2/(Td)}, \qquad \langle \vec{\psi}_n \cdot \vec{\psi}_m\rangle = \delta_{nm}, \quad n,m \in \mathbb{N}. \tag{18}$$

The components $(\mathbf{T}\vec{\psi}_n)_j$, $j = 1,\ldots,d$, of the vector $\mathbf{T}\vec{\psi}_n$ and its norm $\|\mathbf{T}\vec{\psi}_n\|$ are given by

$$(\partial_t\vec{\psi}_n)_j(t) = [\beta(n+j)\pi/T]\cos((n+j)\pi t/T), \quad \|\mathbf{T}\vec{\psi}_n\|^2 = \frac{1}{d}\sum_j [(n+j)\pi/T]^2. \tag{19}$$

Therefore, the norm of the members of the set $\{\mathbf{T}\vec{\psi}_n\}$ grows arbitrarily large as $n \to \infty$. This clearly demonstrates the unboundedness of the operator $\mathbf{T}$ on $\mathscr{H}_{\mathcal{T}}$.

The above analysis demonstrates that the domain $D(\mathbf{T})$ of the unbounded operator $\mathbf{T}$ is defined only on a proper subset of $\mathscr{H}_{\mathcal{T}}$, i.e. $D(\mathbf{T}) \subset \mathscr{H}_{\mathcal{T}}$. However, $D(\mathbf{T})$ can be defined as a *dense* subset of $\mathscr{H}_{\mathcal{T}}$ such that $\mathbf{T}$ is bounded [31, 34]. Toward this goal, consider the class $\mathscr{A}_{\mathcal{T}}$ of all functions $\xi \in L^2(\mathcal{T})$ such that $\xi(t)$ is *absolutely continuous* [32] on the interval $\mathcal{T}$ and has a derivative $\xi'(t)$ belonging to $L^2(\mathcal{T})$, i.e. [34, 32]

$$\mathscr{A}_{\mathcal{T}} = \left\{ \xi \in L^2(\mathcal{T}) \;\middle|\; \xi(t) = c + \int_0^t g(\tau)d\tau, \quad g \in L^2(\mathcal{T}) \right\}, \tag{20}$$

where the constant c and function $g(t)$ are arbitrary. Now, consider the set $\tilde{\mathscr{A}}_{\mathcal{T}}$ of all functions $\xi \in \mathscr{A}_{\mathcal{T}}$ that satisfy the periodic initial condition $\xi(0) = \xi(T)$, i.e. functions ξ satisfying the properties of equation (20) with $\int_0^T g(\tau)d\tau = 0$. To illustrate some important ideas later in this work, we also consider the set $\hat{\mathscr{A}}_{\mathcal{T}}$ of all functions $\xi \in \mathscr{A}_{\mathcal{T}}$ that satisfy the Dirichlet initial condition $\xi(0) = \xi(T) = 0$, i.e. functions ξ satisfying the properties of equation (20) with $c = 0$ and $\int_0^T g(\tau)d\tau = 0$. More concisely,

$$\tilde{\mathscr{A}}_{\mathcal{T}} = \{\xi \in \mathscr{A}_{\mathcal{T}} \,|\, \xi(0) = \xi(T)\}, \quad \hat{\mathscr{A}}_{\mathcal{T}} = \{\xi \in \mathscr{A}_{\mathcal{T}} \,|\, \xi(0) = \xi(T) = 0\}. \tag{21}$$

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 $L^2(\mathcal{T})$ [34]. It follows that the function space $\mathscr{F}_{\mathcal{T}} = \otimes_{n=1}^d \tilde{\mathscr{A}}_{\mathcal{T}}$ is everywhere dense in $\mathscr{H}_{\mathcal{T}}$ and $\mathscr{F}_{\mathcal{T}} \otimes \mathscr{H}_{\mathcal{V}}$ is a dense subset of the Hilbert space $\mathscr{H}_{\mathcal{T}\mathcal{V}}$. Moreover, as a linear operator acting on the function space $\mathscr{F}_{\mathcal{T}}$, by construction, $\mathbf{T}$ is bounded in operator norm. We are now in a position to prove Theorem 2.1.

Proof of Theorem 2.1. As a linear operator acting on the function space $\mathscr{F}_{\mathcal{T}} \otimes \mathscr{H}_{\mathcal{V}}$, by construction, $\boldsymbol{\sigma} = \boldsymbol{\kappa} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ is bounded in operator norm. Recall from (12) that $\vec{J}_k = \boldsymbol{\sigma}\vec{E}_k$ with $\vec{E}_k = \vec{\nabla}\chi_k + \vec{e}_k$. It is clear that $\boldsymbol{\sigma}\vec{e}_k = \boldsymbol{\kappa}\vec{e}_k$, and is bounded by equation (17). Consequently, if $\vec{\nabla}\chi_k \in \mathscr{F}_{\mathcal{T}} \otimes \mathscr{H}_{\mathcal{V}}$ then $\vec{J}_k$ is Lebesgue measurable and also bounded in norm on $\mathscr{H}_{\mathcal{T}\mathcal{V}}$. We have already established that $\vec{\nabla}\chi_k \in \mathscr{H}_{\mathcal{T}} \otimes \mathscr{H}_\times$. Therefore, this and equation (7) suggest that we consider the curl-free, mean-zero vector field $\vec{\nabla}\chi_k$ as a member of the function space $\mathscr{F} \subset \mathscr{F}_{\mathcal{T}} \otimes \mathscr{H}_{\mathcal{V}}$,

$$\mathscr{F} = \{\vec{\xi} \in \mathscr{F}_{\mathcal{T}} \otimes \mathscr{H}_\times \mid \langle \vec{\xi}\rangle = 0\}, \tag{22}$$

which will be used extensively. We stress that $\mathscr{F}$ is *not* a Hilbert space, and is instead a dense subset of the Hilbert space $\mathscr{H}_{\mathcal{T}} \otimes \mathscr{H}_{\times}$. We will henceforth assume that $\vec{\nabla}\chi_k \in \mathscr{F}$. In the case of a time-independent velocity field $\vec{u}$ we set $\mathscr{F}_{\mathcal{T}} = \emptyset$ in (22), so that $\vec{\xi} \in \mathscr{F}$ implies $\vec{\xi} \in \mathscr{H}_{\times}$ with $\langle \vec{\xi} \rangle = 0$. To summarize, since $\boldsymbol{\sigma}$ is bounded on $\mathscr{F}$ and $\vec{\nabla}\chi_k \in \mathscr{F}$, we have that the divergence-free vector field $\vec{J}_k = \boldsymbol{\sigma}\vec{E}_k$ is also bounded $\|\vec{J}_k\| < \infty$, thus $\vec{J}_k \in \mathscr{H}_{\mathcal{T}} \otimes \mathscr{H}_{\bullet}$.

By the mutual orthogonality of the Hilbert spaces $\mathscr{H}_{\times}$ and $\mathscr{H}_{\bullet}$ in equation (16), $\vec{\nabla}\chi_k \in \mathscr{F}$, $\vec{J}_k \in \mathscr{H}_{\mathcal{T}} \otimes \mathscr{H}_{\bullet}$, and Fubini's theorem [12] imply that $\langle \vec{J}_j \cdot \vec{\nabla}\chi_k \rangle = 0$ for every $j, k = 1, \ldots, d$. This is trivially satisfied in the case of a time-independent velocity field $\vec{u}$, since in this case $\boldsymbol{\sigma} = \boldsymbol{\kappa}$ is bounded so that $\vec{J}_j \in \mathscr{H}_{\bullet}$ for $\vec{\nabla}\chi_k \in \mathscr{F}$. In either case, as $\vec{E}_k = \vec{\nabla}\chi_k + \vec{e}_k$, we have $\langle \vec{J}_j \cdot \vec{e}_k \rangle = \langle \vec{J}_j \cdot \vec{E}_k \rangle$. Equations (12) and (13) then imply that the components $\sigma^*_{jk} = \boldsymbol{\sigma}^* \vec{e}_j \cdot \vec{e}_k = \langle \boldsymbol{\sigma}\vec{E}_j \cdot \vec{e}_k \rangle$ of the effective tensor $\boldsymbol{\sigma}^*$ can be expressed as $\sigma^*_{jk} = \langle \boldsymbol{\sigma}\vec{E}_j \cdot \vec{E}_k \rangle$, with $\boldsymbol{\sigma} = \varepsilon \mathbf{I} + \mathbf{S}$ and $\mathbf{S} = \mathbf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$. Consequently,

$$\sigma^*_{jk} = \varepsilon \langle \vec{E}_j \cdot \vec{E}_k \rangle + \langle \mathbf{S}\vec{E}_j \cdot \vec{E}_k \rangle. \tag{23}$$

The property $\langle \vec{\nabla}\chi_k \rangle = 0$ in (7), and equation (9) together imply that

$$\varepsilon \langle \vec{E}_j \cdot \vec{E}_k \rangle = \varepsilon [\langle \vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k \rangle + \langle \vec{\nabla}\chi_j \cdot \vec{e}_k \rangle + \langle \vec{e}_j \cdot \vec{\nabla}\chi_k \rangle + \langle \vec{e}_j \cdot \vec{e}_k \rangle] = \varepsilon (\langle \vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k \rangle + \delta_{jk}) = \kappa^*_{jk}. \tag{24}$$

From the definition of $\mathbf{S} = \mathbf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ in equation (9) we have that $\mathbf{S}\vec{e}_j = \mathbf{H}\vec{e}_j$. Consequently, $\langle \mathbf{S}\vec{e}_j \cdot \vec{e}_k \rangle = \langle \mathbf{H}\vec{e}_j \cdot \vec{e}_k \rangle = 0$, since by equation (17) the matrix $\mathbf{H}$ is (component-wise) mean-zero. Also, by the definition $\vec{u} = \vec{\nabla} \cdot \mathbf{H}$ in (3) and the periodicity of $\mathbf{H}$ and χ_k, we also have $\langle \mathbf{H}\vec{e}_j \cdot \vec{\nabla}\chi_k \rangle = -\langle u_j \chi_k \rangle$ via integration by parts. Therefore, by the skew-symmetry of $\mathbf{S}$ on $\mathscr{F}$, the symmetries $\kappa^*_{kj} = \kappa^*_{jk}$ and $\alpha^*_{kj} = -\alpha^*_{jk}$, and equations (9), (A-12), and (A-13), we have

$$\begin{aligned} \langle \mathbf{S}\vec{E}_j \cdot \vec{E}_k \rangle &= \langle \mathbf{S}\vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k \rangle + \langle \mathbf{S}\vec{\nabla}\chi_j \cdot \vec{e}_k \rangle + \langle \mathbf{S}\vec{e}_j \cdot \vec{\nabla}\chi_k \rangle + \langle \mathbf{S}\vec{e}_j \cdot \vec{e}_k \rangle \\ &= \alpha^*_{jk} - \langle \vec{\nabla}\chi_j \cdot \mathbf{H}\vec{e}_k \rangle + \langle \mathbf{H}\vec{e}_j \cdot \vec{\nabla}\chi_k \rangle \\ &= \alpha^*_{jk} + \langle \chi_j u_k \rangle - \langle u_j \chi_k \rangle \\ &= \alpha^*_{jk} + [\alpha^*_{kj} + \kappa^*_{kj} - \varepsilon\delta_{kj}] - [\alpha^*_{jk} + \kappa^*_{jk} - \varepsilon\delta_{jk}] \\ &= -\alpha^*_{jk}. \end{aligned} \tag{25}$$

In summary, from equations (23)–(25) and the symmetries $\kappa^*_{jk} = \kappa^*_{kj}$ and $\alpha^*_{jk} = -\alpha^*_{kj}$ we have that

$$\sigma^*_{jk} = \kappa^*_{jk} - \alpha^*_{jk} = \kappa^*_{kj} + \alpha^*_{kj} = \mathcal{K}^*_{kj}\,, \tag{26}$$

which is equivalent to equation (14). This concludes our proof of Theorem 2.1 $\square$.

We conclude this section with a derivation of the following resolvent formula for $\vec{\nabla}\chi_k$, involving the orthogonal projection operator $\boldsymbol{\Gamma}_{\times} = \vec{\nabla}(\Delta^{-1})\vec{\nabla}\cdot$ onto curl-free fields in (16),

$$\vec{\nabla}\chi_j = (\varepsilon\mathbf{I} + \mathbf{A})^{-1}\vec{g}_j = (\varepsilon\mathbf{I} + \imath\mathbf{M})^{-1}\vec{g}_j, \quad \mathbf{A} = \boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}, \quad \mathbf{M} = -\imath\mathbf{A}, \quad \vec{g}_j = -\boldsymbol{\Gamma}\mathbf{H}\vec{e}_j, \tag{27}$$

where $\imath = \sqrt{-1}$ and we have defined $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}_{\times}$ for notational simplicity. Equation (27) follows from applying the integro-differential operator $\vec{\nabla}(\Delta^{-1})$ to $\vec{\nabla} \cdot \boldsymbol{\sigma}\vec{E}_j = 0$ in equation (12), with $\vec{E}_j = \vec{\nabla}\chi_j + \vec{e}_j$ and $\boldsymbol{\sigma} = \varepsilon\mathbf{I} + \mathbf{S}$, yielding

$$\boldsymbol{\Gamma}(\varepsilon\mathbf{I} + \mathbf{S})\vec{\nabla}\chi_j = -\boldsymbol{\Gamma}\mathbf{H}\vec{e}_j, \tag{28}$$

since $\boldsymbol{\Gamma}\vec{e}_j = 0$ and $\mathbf{S}\vec{e}_j = \mathbf{H}\vec{e}_j$. The equivalence of equations (27) and (28) can be seen by noting that $\vec{\nabla}\chi_j \in \mathscr{F}$ implies $\boldsymbol{\Gamma}\vec{\nabla}\chi_j = \vec{\nabla}\chi_j$. We stress that the property $\boldsymbol{\Gamma}\vec{\nabla}\chi_j = \vec{\nabla}\chi_j$ implies that $\mathbf{A}\vec{\nabla}\chi_j = \boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}\vec{\nabla}\chi_j = \boldsymbol{\Gamma}\mathbf{S}\vec{\nabla}\chi_j = (\boldsymbol{\Gamma}\mathbf{H} - \boldsymbol{\Delta}^{-1}\mathbf{T})\vec{\nabla}\chi_j$.

It is worth mentioning that taking the $\ell^2(\mathbb{C}^N)$ inner-product of both sides of equation (28) with $\vec{\nabla}\chi_k$, averaging, using the properties $\boldsymbol{\Gamma}\vec{\nabla}\chi_j = \vec{\nabla}\chi_j$ and $\langle \boldsymbol{\Gamma}\vec{\xi} \cdot \vec{\zeta} \rangle = \langle \vec{\xi} \cdot \boldsymbol{\Gamma}\vec{\zeta} \rangle$ for $\vec{\xi}, \vec{\zeta} \in \mathscr{H}_{\mathcal{V}}$, and integrating by parts, yields equation (A-13). Moreover, the condition $\langle \vec{J}_j \cdot \vec{\nabla}\chi_k \rangle = 0$ is also equivalent to equation (A-13).

In Section A-1.3 we show that $\mathbf{A}$ in (27) acts as an anti-symmetric linear operator on the Hilbert space $\mathscr{H}_{\mathcal{TV}}$, $\langle \mathbf{A}\vec{\xi} \cdot \vec{\zeta} \rangle = \langle \vec{\xi} \cdot \mathbf{A}^*\vec{\zeta} \rangle = -\langle \vec{\xi} \cdot \mathbf{A}\vec{\zeta} \rangle$. 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 [34]. Consequently, due to the sesquilinearity of the $\mathscr{H}_{\mathcal{TV}}$-inner-product, $\mathbf{M} = -\imath\mathbf{A}$ acts as a *symmetric* operator, $\mathbf{M}^* = \mathbf{M}$ [31, 34]. Moreover, on the function space $\mathscr{F}$, $\mathbf{A}$ is a *maximal* normal operator and $\mathbf{M}$ is *self-adjoint* [34]. In Section 4 we examine these properties of $\mathbf{A}$ and $\mathbf{M}$ in more detail and demonstrate how equation (27) and the spectral theory of such operators lead to integral representations for the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of $\boldsymbol{\mathcal{K}}^*$.

4. Integral representations of the effective diffusivity

In this section, we employ the Hilbert space formulation of the effective parameter problem discussed in Section 3 above, to provide integral representations for the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$, 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 $\mathbf{A} = \mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}$ on $\mathscr{F}$, or equivalently the self-adjoint operator $\mathbf{M} = -\imath\mathbf{A}$, and follow from the spectral theorem for such linear operators [31, 34] and the resolvent formula for $\vec{\nabla}\chi_k$ given in equation (27). The derivation of these integral representations for $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ is the topic of Section 4.1. In Section 4.2 we discuss an important alternate formulation of the effective parameter problem, where the spatial Hilbert space $\mathscr{H}_\times$ is replaced by a Sobelov space $\mathcal{H}^1_{\mathcal{V}}$. In Section 4.3 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 4.4 we review this theory and provide an explicit derivation of the discrete component of these integrals, by eigenfunction expansion. In Sections 4.5 and 4.6 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 7 to formulate an efficient and stable numerical algorithm for the explicit computation of $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ for model velocity fields $\vec{u}$, by the direct computation of $\mathrm{d}\boldsymbol{\mu}$ in terms of the eigenvalues and eigenvectors of $\mathbf{A}$.

4.1. General infinite dimensional setting - curl free.

In the general Hilbert space setting, there are significant differences in the theory between the case of steady flows, where $\mathbf{S} = \mathbf{H}$ is *bounded* on the Hilbert space $\mathscr{H}_{\mathcal{V}}$, and the case of dynamic flows, where $\mathbf{S} = \mathbf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$ is *unbounded* on the Hilbert space $\mathscr{H}_{\mathcal{TV}}$, as discussed in Section 3. It is therefore natural to start our discussion with a more detailed look into this distinction, in the present context. Since $\mathbf{\Gamma}$ is an orthogonal projector from $\mathscr{H}_{\mathcal{V}}$ to $\mathscr{H}_\times$, it is bounded by unity in operator norm $\|\mathbf{\Gamma}\| \le 1$ on $\mathscr{H}_{\mathcal{V}}$ and $\|\mathbf{\Gamma}\| = 1$ on $\mathscr{H}_\times$ [31, 34]. Therefore by (17), in the case of steady flows, the operator $\mathbf{A} = \mathbf{\Gamma}\mathbf{H}\mathbf{\Gamma}$ is bounded on the Hilbert space $\mathscr{H}_{\mathcal{V}}$, with $\|\mathbf{A}\| \le \|\mathbf{H}\| < \infty$. 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 $\langle \mathbf{M}\vec{\xi}, \vec{\zeta} \rangle = \langle \vec{\xi}, \mathbf{M}^*\vec{\zeta} \rangle$, and is also a bounded operator on $\mathscr{H}_{\mathcal{V}}$ with $\|\mathbf{M}^*\| = \|\mathbf{M}\|$ [31]. Consequently, they have identical domains,

$$D(\mathbf{M}) = D(\mathbf{M}^*), \tag{29}$$

which are the entire space, $D(\mathbf{M}) = D(\mathbf{M}^*) = \mathscr{H}_{\mathcal{V}}$. In Section A-1.3 we show that $\mathbf{M}$ is symmetric,

$$\langle \mathbf{M}\vec{\xi} \cdot \vec{\zeta} \rangle = \langle \vec{\xi} \cdot \mathbf{M}\vec{\zeta} \rangle, \ \text{ for all } \ \vec{\xi}, \vec{\zeta} \in D(\mathbf{M}). \tag{30}$$

By definition [31, 34], the two properties (29) and (30) 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 [31] states, if the operator $\mathbf{M}$ satisfies equation (30) for *every* $\vec{\xi}, \vec{\zeta} \in \mathscr{H}_{\mathcal{V}}$, then $\mathbf{M}$ is bounded on $\mathscr{H}_{\mathcal{V}}$. This suggests that, in the time-dependent case when $\mathbf{M}$ is unbounded on the Hilbert space $\mathscr{H}_{\mathcal{T}\mathcal{V}}$, it is defined as a self-adjoint operator only on a proper subset of $\mathscr{H}_{\mathcal{T}\mathcal{V}}$. However, as discussed in Section 3, the domain $D(\mathbf{M})$ can be defined as a *dense* subset of $\mathscr{H}_{\mathcal{T}\mathcal{V}}$ such that $\mathbf{M}$ is bounded. Moreover, on this domain, $\mathbf{M}$ can be extended to a *closed* symmetric operator [31, 34]. Although even in this case, in general [31], 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 [31], which provides the existence of the promised integral representation for $\boldsymbol{\mathcal{K}}^*$, 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 $\mathbf{\Gamma}$ is bounded on $\mathscr{H}_{\mathcal{V}}$ and $\mathbf{M} = -\imath\mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}$, our discussion in Section 3 indicates that the unboundedness of $\mathbf{M}$ on $\mathscr{H}_{\mathcal{T}\mathcal{V}}$ is due to the unboundedness of the underlying operator $\mathbf{T}$ on the Hilbert space $\mathscr{H}_{\mathcal{T}}$. 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 (20) and (21), which are everywhere dense in $L^2(\mathcal{T})$ [34]. 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 $\hat{B}$ [34]. 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 $\imath\mathbf{T} = \imath\partial_t\mathbf{I}$ with domain $D(\mathbf{T}) = \mathscr{F}_{\mathcal{T}} = \otimes_{n=1}^{d}\tilde{\mathscr{A}_{\mathcal{T}}}$ is self-adjoint. This is seen as follows. By noting that $\imath\mathbf{T}\vec{\xi} = (\tilde{B}\xi_1, \ldots, \tilde{B}\xi_d)$ and, for all $\vec{\xi}, \vec{\zeta} \in \mathscr{F}_{\mathcal{T}}$ with components $\xi_j, \zeta_j \in \tilde{\mathscr{A}_{\mathcal{T}}}$, $j = 1, \ldots, d$, the self-adjointness of $\tilde{B}$ implies that $\mathbf{T}$ is symmetric, $\mathbf{T} = \mathbf{T}^*$, on $\mathscr{F}_{\mathcal{T}}$,

$$\langle \mathbf{T}\vec{\xi} \cdot \vec{\zeta} \rangle = \sum_j \langle \tilde{B}\xi_j, \zeta_j \rangle_2 = \sum_j \langle \xi_j, \tilde{B}\zeta_j \rangle_2 = \langle \vec{\xi} \cdot \mathbf{T}\vec{\zeta} \rangle, \tag{31}$$

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 $D(\mathbf{T}) = D(\mathbf{T}^*) = \mathscr{F}_{\mathcal{T}}$, i.e. $\mathbf{T} \equiv \mathbf{T}^*$ on $\mathscr{F}_{\mathcal{T}}$. Consequently, $\mathbf{T}$ is a bounded self-adjoint linear operator on the function space $\mathscr{F}_{\mathcal{T}}$.

We now summarize what we have discussed so far, and discuss the implications thereof. We have discussed that the operators $(\boldsymbol{\Delta}^{-1})$ and $\mathbf{\Gamma}$ are bounded on the Hilbert space $\mathscr{H}_{\mathcal{V}}$. In Section A-1.3 we show that they are also symmetric, hence self-adjoint on $\mathscr{H}_{\mathcal{V}}$. Due to the sesquilinearity of the $\mathscr{H}_{\mathcal{T}\mathcal{V}}$-inner-product, and equations (17) and (3) with $\mathbf{H}^* = \mathbf{H}^T$, the operator $\imath\mathbf{H}$ is bounded and symmetric, hence self-adjoint on the Hilbert space $\mathscr{H}_{\mathcal{T}\mathcal{V}}$. Consequently, the operator $\imath\mathbf{\Gamma}\mathbf{H}\mathbf{\Gamma}$ is also self-adjoint on $\mathscr{H}_{\mathcal{T}\mathcal{V}}$. The differential and integral operators $\imath\mathbf{T}$ and $(\boldsymbol{\Delta}^{-1})$ are bounded on the function space $\mathscr{F}_{\mathcal{T}}$ and Hilbert space $\mathscr{H}_{\mathcal{V}}$, respectively, and they are consequently commutable operations on the function space $\mathscr{F}_{\mathcal{T}} \times \mathscr{H}_{\mathcal{V}}$ [12]. Moreover, as $\imath\mathbf{T}$ and $(\boldsymbol{\Delta}^{-1})$ are self-adjoint on $\mathscr{F}_{\mathcal{T}}$ and $\mathscr{H}_{\mathcal{V}}$, respectively, the operator $\imath(\boldsymbol{\Delta}^{-1})\mathbf{T}$, hence $\imath\mathbf{\Gamma}[(\boldsymbol{\Delta}^{-1})\mathbf{T}]\mathbf{\Gamma}$ is self-adjoint on $\mathscr{F}_{\mathcal{T}} \times \mathscr{H}_{\mathcal{V}}$. It is now clear that the operator $\mathbf{M} = \imath\mathbf{\Gamma}\mathbf{S}\mathbf{\Gamma}$, with $\mathbf{S} = \mathbf{H} - (\boldsymbol{\Delta}^{-1})\mathbf{T}$, is self-adjoint on $\mathscr{F}_{\mathcal{T}} \times \mathscr{H}_{\mathcal{V}}$. Finally, since $\mathbf{M} = -\imath\mathbf{A}$ is self-adjoint on $\mathscr{F}_{\mathcal{T}} \times \mathscr{H}_{\mathcal{V}}$ and an operator is self-adjoint if and only if it is a maximal normal operator [34], we have that $\mathbf{A}$ is a maximal normal operator on $\mathscr{F}_{\mathcal{T}} \times \mathscr{H}_{\mathcal{V}}$. In view of the resolvent formulas for $\vec{\nabla}\chi_j \in \mathscr{F}$ in (27) involving $\mathbf{M}$ and $\mathbf{A}$, we will henceforth take the domain of these operators to be $D(\mathbf{A}) = D(\mathbf{M}) = \mathscr{F}$ in (22), which is a *closed* subset of $\mathscr{F}_{\mathcal{T}} \times \mathscr{H}_{\mathcal{V}}$.

In terms of a general, maximal normal operator $\mathbf{N}$ on $\mathscr{F}$ satisfying $\mathbf{N}\mathbf{N}^* = \mathbf{N}^*\mathbf{N}$, the spectral theorem states that $\mathbf{N}$ can be decomposed as $\mathbf{N} = \mathbf{H}_1 + \imath\mathbf{H}_2$, where $\mathbf{H}_1$ and $\mathbf{H}_2$ are self-adjoint and commute on $\mathscr{F}$ [34]. Moreover, there is a one-to-one correspondence between $\mathbf{H}_n$, $n = 1, 2$, and a family $\{\mathbf{Q}_n(\lambda)\}$, $-\infty<\lambda<\infty$, of self-adjoint projection operators - the resolution of the identity - with domain $\mathscr{F}$ which satisfies $\lim_{\lambda\to-\infty}\mathbf{Q}_n(\lambda)=0$, $\lim_{\lambda\to+\infty}\mathbf{Q}_n(\lambda)=\mathbf{I}$, and the $\mathbf{Q}_n(\lambda)$, $n=1,2$, commute [31, 34]. 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 $\mathbf{Q}(z)\to\mathbf{I}$ when $\mathrm{Re}(z)\to+\infty$ and when $\mathrm{Im}(z)\to+\infty$ [34].

The spectral theorem also provides an operational calculus in Hilbert space which yields integral representations associated with $\mathbf{Q}(z)$-measurable functions of $\mathbf{N}$ [34]. The details are as follows. Let $\vec{\xi},\vec{\zeta}\in\mathscr{F}$ and consider the *complex-valued* function $\mu_{\xi\zeta}(z)=\langle\mathbf{Q}(z)\vec{\xi}\cdot\vec{\zeta}\rangle$, $\vec{\xi}\neq\vec{\zeta}$. By the sesquilinearity of the inner-product and the self-adjointness of the projection operator $\mathbf{Q}(z)$ we have $\mu_{\zeta\xi}(z)=\overline{\mu}_{\xi\zeta}(z)$, where $\overline{\mu}_{\xi\zeta}$ denotes the complex conjugate of $\mu_{\xi\zeta}$. Moreover, the function $\mu_{\xi\xi}$ is real-valued and positive $\mu_{\xi\xi}(z)=\langle\mathbf{Q}(z)\vec{\xi}\cdot\vec{\xi}\rangle=\langle\mathbf{Q}(z)\vec{\xi}\cdot\mathbf{Q}(z)\vec{\xi}\rangle=\|\mathbf{Q}(z)\vec{\xi}\|^2$. We associate with these functions of *bounded variation* Radon–Stieltjes measures $\mathrm{d}\mu_{\xi\zeta}(z)$ and $\mathrm{d}\mu_{\xi\xi}(z)$ [34]

$$\mathrm{d}\mu_{\xi\zeta}(z)=\mathrm{d}\langle\mathbf{Q}(z)\vec{\xi}\cdot\vec{\zeta}\rangle,\quad \vec{\xi}\neq\vec{\zeta},\qquad \mathrm{d}\mu_{\xi\xi}(z)=\mathrm{d}\|\mathbf{Q}(z)\vec{\xi}\|^2. \tag{32}$$

Let $F(z)$ be an arbitrary complex-valued function and denote by $\mathscr{D}(F)$ the set of all $\vec{\xi}\in\mathscr{F}$ such that $F\in L^2(\mu_{\xi\xi})$, i.e. $F(z)$ is square integrable with respect to the measure $\mathrm{d}\mu_{\xi\xi}$. 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 [34]

$$\langle F(\mathbf{N})\vec{\xi}\cdot\vec{\zeta}\rangle=\int_I\overline{F(z)}\,\mathrm{d}\mu_{\xi\zeta}(z),\qquad\forall\vec{\xi}\in\mathscr{D}(F),\ \vec{\zeta}\in\mathscr{F} \tag{33}$$
$$\langle F(\mathbf{N})\vec{\xi}\cdot G(\mathbf{N})\vec{\zeta}\rangle=\int_I\overline{F}(z)G(z)\,\mathrm{d}\mu_{\xi\zeta}(z),\quad\forall\vec{\xi}\in\mathscr{D}(F),\ \vec{\zeta}\in\mathscr{D}(G),$$

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 $\|F(\mathbf{N})\vec{\xi}\|^2$ follows from the second formula in (33) with $G=F$ and $\vec{\xi}=\vec{\zeta}$, and involves the measure $\mathrm{d}\mu_{\xi\xi}$ in (32) [34]. The domain of integration I in (33) 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 $I\subseteq(-\infty,\infty)\times(-\imath\infty,\imath\infty)$ [31, 34]. We will discuss the properties of $\Sigma(\mathbf{N})$ in detail in Section 6.

The spectral theorem of equation (33) for the maximal normal operator $\mathbf{N}$ on $\mathscr{F}$ generalizes that for self-adjoint and maximal anti-symmetric operators, with purely real and imaginary spectrum, respectively. More specifically, the case $F(z)=z=\lambda_1+\imath\lambda_2$ corresponds to $F(\mathbf{N})=\mathbf{H}_1+\imath\mathbf{H}_2$ with $I\subseteq(-\infty,\infty)\times(-\imath\infty,\imath\infty)$ and $\mathbf{Q}(z)=\mathbf{Q}_1(\mathrm{Re}(z))\mathbf{Q}_2(\mathrm{Im}(z))$, the case $F(z)=\mathrm{Re}(z)$ corresponds to the self-adjoint operator $F(\mathbf{N})=\mathbf{H}_1$ 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 $F(\mathbf{N})=\imath\mathbf{H}_2$ with $I\subseteq(-\imath\infty,\imath\infty)$ and $\mathbf{Q}(z)=\mathbf{Q}_2(\mathrm{Im}(z))$ [34]. We now apply the spectral theorem to equations (9) and (27) to provide Radon–Stieltjes integral representations for the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$, for both cases of time-independent and time-dependent velocity fields $\vec{u}$. These representations are summarized by the following theorem.

Theorem 4.1. *Let $z=\imath\lambda$, $\vec{g}_j=-\boldsymbol{\Gamma}\mathbf{H}\vec{e}_j$ be defined as in (27), 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 (27), with domain $\mathscr{F}$ defined in (22). Define the matrix-valued function $\boldsymbol{\mu}(\lambda)$ with complex-valued off-diagonal components $\mu_{jk}(\lambda)=\langle\mathbf{Q}_2(\lambda)\vec{g}_j\cdot\vec{g}_k\rangle$ for $j\neq k=1,\dots,d$, with $\mu_{kj}=\overline{\mu}_{jk}$, and positive diagonal components $\mu_{kk}(\lambda)=\|\mathbf{Q}_2(\lambda)\vec{g}_k\|^2$. Moreover, consider the real-valued functions*

$$\mathrm{Re}\,\mu_{jk}(\lambda)=\frac{1}{2}\left(\mu_{jk}(\lambda)+\overline{\mu}_{jk}(\lambda)\right),\quad \mathrm{Im}\,\mu_{jk}(\lambda)=\frac{1}{2\,\imath}\left(\mu_{jk}(\lambda)-\overline{\mu}_{jk}(\lambda)\right). \tag{34}$$

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* κ^*_{jk} *and* α^*_{jk}, $j,k=1,\dots,d$, *of the effective tensors* $\boldsymbol{\kappa}^*$ *and* $\boldsymbol{\alpha}^*$ *defined in equation* (9), *given by*

$$\kappa^*_{jk} = \varepsilon\left(\delta_{jk} + \int_{-\infty}^{\infty} \frac{\mathrm{dRe}\,\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\right), \qquad \alpha^*_{jk} = \int_{-\infty}^{\infty} \frac{\lambda\,\mathrm{dIm}\,\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\,. \tag{35}$$

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* $\|\mathbf{A}\| \le \|\mathbf{H}\| < \infty$ *in the case of a time-independent velocity field* $\vec{u}$ [31].

A key feature of the integral representations for $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ in (35) is that parameter information in ε is *separated* from the geometry and dynamics of the velocity field $\vec{u}$, which are encapsulated in the underlying spectral measure $\mathrm{d}\boldsymbol{\mu}$. In Section 4.4 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 5 to calculate κ^*_{jk} and α^*_{jk} for a large class of velocity fields $\vec{u}$. Furthermore, in Section 6 these important properties of the integrals in (35) lead to asymptotic behavior of $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ 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 4.1. We first note that from $\vec{\nabla}\chi_k \in \mathscr{F}$ we have $\vec{\nabla}\chi_k = \boldsymbol{\Gamma}\vec{\nabla}\chi_k$, so that α^*_{jk} in equation (9) can re-expressed as $\alpha^*_{jk} = \langle \mathbf{S}\vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k\rangle = \langle \boldsymbol{\Gamma}\mathbf{S}\boldsymbol{\Gamma}\vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k\rangle = \langle \mathbf{A}\vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k\rangle$, where we have used that $\boldsymbol{\Gamma}$ is self-adjoint on $\mathscr{F}$. From this and (27), equation (9) can be rewritten as

$$\kappa^*_{jk} = \varepsilon\left(\delta_{jk} + \langle(\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_j \cdot (\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_k\rangle\right), \quad \alpha^*_{jk} = \langle \mathbf{A}(\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_j \cdot (\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_k\rangle, \tag{36}$$

where $\vec{g}_k = -\boldsymbol{\Gamma}\mathbf{H}\vec{e}_k$. The integral representations for κ^*_{jk} and α^*_{jk} in (35) follow from equations (33) and (36), and the symmetries $\langle\vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k\rangle = \langle\vec{\nabla}\chi_k \cdot \vec{\nabla}\chi_j\rangle$ and $\langle\mathbf{A}\vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k\rangle = \langle\vec{\nabla}\chi_k \cdot \mathbf{A}\vec{\nabla}\chi_j\rangle$, since $\vec{\nabla}\chi_k$ and $\mathbf{A}\vec{\nabla}\chi_k$ are real-valued. We prove the validity of (35) by showing that the conditions of the spectral theorem of equation (33) are satisfied for the functionals in (36) and then employing these symmetries.

We first show that $\vec{g}_k \in \mathscr{F}$ for all $k=1,\dots,d$. Indeed, the orthogonality of the projection operators $\boldsymbol{\Gamma}_\times = \boldsymbol{\Gamma}$ and $\boldsymbol{\Gamma}_0$ defined in equation (16) implies that the vector field $\vec{g}_k(t,\cdot) = \boldsymbol{\Gamma}\mathbf{H}(t,\cdot)\vec{e}_k$ is curl-free and mean-zero for each $t \in \mathcal{T}$ fixed, and by equation (17) we have $\|\vec{g}_k\| \le \|\mathbf{H}\| < \infty$. This and the periodicity of $\mathbf{H}$ implies that $\vec{g}_k(t,\cdot) \in \mathscr{H}_\times$, and by Fubini's theorem [12] we have $\langle\vec{g}_k\rangle = 0$. By the uniform boundedness of $\boldsymbol{\Gamma}$ on $\mathscr{H}_\mathcal{V}$ and equation (17), we also have [12] that $\|\mathbf{T}\vec{g}_k\| = \|\mathbf{T}\boldsymbol{\Gamma}\mathbf{H}\vec{e}_k\| = \|\boldsymbol{\Gamma}\mathbf{T}\mathbf{H}\vec{e}_k\| \le \|\mathbf{T}\mathbf{H}\| < \infty$. Therefore $\vec{g}_k(\cdot,\vec{x}), \mathbf{T}\vec{g}_k(\cdot,\vec{x}) \in \mathscr{H}_\mathcal{T}$ for each $\vec{x} \in \mathcal{V}$ fixed, which implies that $\vec{g}_k(\cdot,\vec{x}) \in \mathscr{F}_\mathcal{T}$. Consequently, $\vec{g}_k \in \mathscr{F}$ for all $k=1,\dots,d$.

Consider the representation for κ^*_{jk} in (36) and define the function $F(z) = (\varepsilon+z)^{-1}$ so that, formally, $\kappa^*_{jk} = \varepsilon(\delta_{jk} + \langle F(\mathbf{A})\vec{g}_j \cdot F(\mathbf{A})\vec{g}_k\rangle)$. Since $\vec{g}_k \in \mathscr{F}$ for all $k=1,\dots,d$, once we establish that $\vec{g}_k \in \mathscr{D}(F)$, i.e. $F \in L^2(\mu_{kk})$, the integral representations for κ^*_{jk}, $j,k=1,\dots,d$, in (35) follow from the second formula in (33) with $F(z) = G(z) = (\varepsilon+z)^{-1}$, $\vec{\xi} = \vec{g}_j$, and $\vec{\zeta} = \vec{g}_k$. 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 $\mu_{jk}(z) = \langle \mathbf{Q}(z)\vec{g}_j \cdot \vec{g}_k\rangle$ is of *bounded variation* when $\vec{g}_j, \vec{g}_k \in \mathscr{F}$, hence $|\mu^0_{jk}| < \infty$ for all $j,k=1,\dots,d$ [34]. We have therefore established that $\vec{g}_k \in \mathscr{D}(F)$ for all $k=1,\dots,d$.

Before we employ the symmetry $\langle\vec{\nabla}\chi_j \cdot \vec{\nabla}\chi_k\rangle = \langle\vec{\nabla}\chi_k \cdot \vec{\nabla}\chi_j\rangle$ to derive the integral representations for κ^*_{kk} and κ^*_{jk} in (35), we note that the condition $\mu^0_{kk} < \infty$ implies that $\vec{g}_k \in \mathscr{D}(F)$ for the function $F(z) = 1$. This leads to an explicit representation of the mass μ^0_{jk} in terms of $\boldsymbol{\Gamma}$ and $\mathbf{H}$, and provides a bound for $|\mu^0_{jk}|$. Indeed, taking $F(z) = 1$ ($F(\mathbf{A}) = \mathbf{I}$), $\vec{\xi} = \vec{g}_j$, and $\vec{\zeta} = \vec{g}_k$ in the first formula of equation (33), the self-adjointness of $\mathbf{\Gamma}$ and $\mathbf{\Gamma}^2=\mathbf{\Gamma}$ on $\mathscr{F}$ implies that

$$\mu^0_{jk}=\int_I \mathrm{d}\mu_{jk}(z)=\int_I \mathrm{d}\langle \mathbf{Q}(z)\vec{g}_j,\vec{g}_k\rangle=\langle \vec{g}_j,\vec{g}_k\rangle=\langle \mathbf{\Gamma}\mathbf{H}\vec{e}_j\cdot\mathbf{\Gamma}\mathbf{H}\vec{e}_k\rangle=\langle \mathbf{H}^T\mathbf{\Gamma}\mathbf{H}\vec{e}_j\cdot\vec{e}_k\rangle. \tag{37}$$

This and equation (17) imply that $|\mu^0_{jk}|\le\|\mathbf{H}\|^2<\infty$ for all $j,k=1,\ldots,d$.

We now derive the integral representations for κ^*_{kk} and κ^*_{jk}, $j\neq k=1,\ldots,d$, displayed in (35). For the function $F(z)=(\varepsilon+z)^{-1}$, we have established above that $\vec{g}_k\in\mathscr{D}(F)$ for all $k=1,\ldots,d$, so that $\kappa^*_{jk}=\varepsilon(\delta_{jk}+\langle F(\mathbf{A})\vec{g}_j\cdot F(\mathbf{A})\vec{g}_k\rangle)$ is well defined in terms of a Radon–Stieltjes integral. Specifically, the second formula in equation (33) with $F(z)=G(z)=(\varepsilon+z)^{-1}$, $\vec{\xi}=\vec{g}_j$, $\vec{\zeta}=\vec{g}_k$, $\mathrm{d}\mu_{\xi\zeta}(z):=\mathrm{d}\mu_{jk}(z)=\mathrm{d}\langle\mathbf{Q}(z)\vec{g}_j\cdot\vec{g}_k\rangle=\mathrm{d}\langle\mathbf{Q}_2(\mathrm{Im}(z))\vec{g}_j\cdot\vec{g}_k\rangle$, and $z=\imath\lambda$ yields

$$\kappa^*_{jk}/\varepsilon-\delta_{jk}=\int_I\frac{\mathrm{d}\mu_{jk}(z)}{\overline{(\varepsilon+z)}(\varepsilon+z)}=\int_I\frac{\mathrm{d}\mu_{jk}(z)}{\varepsilon^2+|z|^2}=\int_{-\imath\infty}^{\imath\infty}\frac{\mathrm{d}\mu_{jk}(\mathrm{Im}(z))}{\varepsilon^2+|\mathrm{Im}(z)|^2}=\int_{-\infty}^{\infty}\frac{\mathrm{d}\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}. \tag{38}$$

Equation (38) establishes the integral representation for κ^*_{kk} in (35), since $\mu_{kk}(z)=\|\mathbf{Q}(z)\vec{g}_k\|^2$ is a positive function so that $\mathrm{Re}\,\mu_{kk}(z)=\mu_{kk}(z)$ and $\mathrm{d}\mu_{kk}(z)=\mathrm{d}\|\mathbf{Q}(z)\vec{g}_k\|^2$ is a *positive measure*. However for $j\neq k$, the function $\mu_{jk}(z)=\langle\mathbf{Q}(z)\vec{g}_j\cdot\vec{g}_k\rangle$ 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 $\vec{\nabla}\chi_k$ is real-valued, the functional $\langle\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle=\langle F(\mathbf{A})\vec{g}_j\cdot F(\mathbf{A})\vec{g}_k\rangle$ is also real-valued, which implies that the final integral in (38) must be representable in terms of a *signed measure* for $j\neq k$. The validity of this follows from the symmetry $\langle\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle=\langle\vec{\nabla}\chi_k\cdot\vec{\nabla}\chi_j\rangle$, so that $2\langle\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle=\langle\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle+\langle\vec{\nabla}\chi_k\cdot\vec{\nabla}\chi_j\rangle$. Therefore, since $\mu_{kj}(\lambda)=\overline{\mu}_{jk}(\lambda)$, by the linearity properties of Radon–Stieltjes integrals [34], for $j\neq k=1,\ldots,d$, equation (38) becomes

$$\kappa^*_{jk}/\varepsilon-\delta_{jk}=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\mathrm{d}(\mu_{jk}(\lambda)+\overline{\mu}_{jk}(\lambda))}{\varepsilon^2+\lambda^2}=\int_{-\infty}^{\infty}\frac{\mathrm{dRe}\,\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\,, \tag{39}$$

which establishes the integral representation for κ^*_{jk} in (35) for $j\neq k$. As anticipated, the integral representation for κ^*_{jk} in equation (35) satisfies $\kappa^*_{kj}=\kappa^*_{jk}$, 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 α^*_{jk}, $j\neq k=1,\ldots,d$, displayed in equation (35). Consider the representation for α^*_{jk} in (36) and define the functions $F(z)=z(\varepsilon+z)^{-1}$ and $G(z)=(\varepsilon+z)^{-1}$ so that, formally, $\alpha^*_{jk}=\langle F(\mathbf{A})\vec{g}_j\cdot G(\mathbf{A})\vec{g}_k\rangle$. We have already established that $\vec{g}_k\in\mathscr{D}(G)$ for all $k=1,\ldots,d$. 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 (17) and (37), the positive measure $\mathrm{d}\mu_{kk}$ has bounded mass $\mu^0_{kk}\le\|\mathbf{H}\|^2<\infty$, which implies that $F\in L^2(\mu_{kk})$ hence $\vec{g}_k\in\mathscr{D}(F)$ for all $k=1,\ldots,d$. Consequently, the functional $\alpha^*_{jk}=\langle F(\mathbf{A})\vec{g}_j\cdot G(\mathbf{A})\vec{g}_k\rangle$ has a well defined meaning in terms of a Radon-Stieltjes integral. Specifically, the second formula in equation (33) with $F(z)=z(\varepsilon+z)^{-1}$, $G(z)=(\varepsilon+z)^{-1}$, $\vec{\xi}=\vec{g}_j$, $\vec{\zeta}=\vec{g}_k$, $\mathrm{d}\mu_{\xi\zeta}(z):=\mathrm{d}\mu_{jk}(z)$ defined as in equation (38), and $z=\imath\lambda$ yields

$$\alpha^*_{jk}=\int_I\frac{\overline{z}\,\mathrm{d}\mu_{jk}(z)}{\varepsilon^2+|z|^2}=\int_{-\imath\infty}^{\imath\infty}\frac{-\imath\,\mathrm{Im}(z)\mathrm{d}\mu_{jk}(\mathrm{Im}(z))}{\varepsilon^2+|\mathrm{Im}(z)|^2}=\int_{-\infty}^{\infty}\frac{-\imath\lambda\,\mathrm{d}\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\,. \tag{40}$$

Similar to the derivation of the integral representation for κ^*_{jk} in (39) when $j\neq k$, we use that $\alpha^*_{jk}=\langle\mathbf{A}\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle=\langle F(\mathbf{A})\vec{g}_j\cdot G(\mathbf{A})\vec{g}_k\rangle$ is real-valued. This implies that we have the symmetry $\langle\mathbf{A}\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle=\langle\vec{\nabla}\chi_k\cdot\mathbf{A}\vec{\nabla}\chi_j\rangle$, so that $2\langle\mathbf{A}\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle=\langle\mathbf{A}\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle+\langle\vec{\nabla}\chi_k\cdot\mathbf{A}\vec{\nabla}\chi_j\rangle$. This, equation (40), $\mu_{kj}(z)=\overline{\mu}_{jk}(z)$, $z=\imath\lambda$, and the linearity properties of Radon–Stieltjes integrals [34] imply that

$$\alpha^*_{jk}=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\lambda\,\mathrm{d}(\imath\,[\overline{\mu}_{jk}(\lambda)-\mu_{jk}(\lambda)])}{\varepsilon^2+\lambda^2}=\int_{-\infty}^{\infty}\frac{\lambda\,\mathrm{dIm}\,\mu_{jk}(\lambda)}{\varepsilon^2+\lambda^2}\,, \tag{41}$$

which establishes the integral representation for α^*_{jk} in (35). As anticipated, the integral representation for α^*_{jk} in equation (35) satisfies $\alpha^*_{kj} = -\alpha^*_{jk}$, since $\mu_{kj}(\lambda) = \overline{\mu}_{jk}(\lambda)$ implies that $\operatorname{Im}\mu_{kj}(\lambda) = -\operatorname{Im}\mu_{jk}(\lambda)$. Moreover, since $\mu_{kk}(\lambda)$ is real-valued so that $\operatorname{Im}\mu_{kk}(\lambda) \equiv 0$, we also have $\alpha^*_{kk} = 0$.

We have already discussed that the domain of integration I of the integral representations in (33) are determined by the spectrum $\Sigma(\mathbf{N})$ of the maximal normal operator $\mathbf{N}$. Hence, the domain of integration in equation (35) is determined by the spectrum $\Sigma(\mathbf{A})$ of the operator $\mathbf{A}$. Although, we were able to take $I \subseteq (-\infty, \infty)$ in (35) because of the properties of the functions $F(z)$, $G(z)$, and $\mu_{jk}(z)$ underlying these integral representations (see equations (38) and (40)). Since the spectral radius of the normal operator $\mathbf{A}$ is given by its norm $\|\mathbf{A}\|$ [31], I can be an unbounded set in the case of a time-dependent velocity field $\vec{u}$ and $I \subseteq [-\|\mathbf{A}\|, \|\mathbf{A}\|]$ with $\|\mathbf{A}\| \leq \|\mathbf{H}\| < \infty$ in the case of a time-independent velocity field. This concludes our proof of Theorem 4.1 $\square$.

4.2. **General infinite dimensional setting - Sobelov.** We now discuss an important corollary of Theorem 4.1 that provides integral representations for $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ in terms of an anti-symmetric operator A, which acts on *scalar-valued* functions. This formulation [29, 6] of the effective parameter problem for $\boldsymbol{\mathcal{K}}^*$ 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 7 to compute the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ for model flows. For the case of a time-independent, continuously differentiable velocity field $\vec{u}$, the operator A is compact on a Sobolev space $\mathcal{H}^1_{\mathcal{V}}$ [6], and a resolvent formula for χ_j involving A has led to [29] a discrete version of the integral representation for $\boldsymbol{\alpha}^*$ displayed in (35). We now show that the conditions of Theorem 4.1 can be modified slightly to generalize this result for $\boldsymbol{\alpha}^*$ to the case of a time-dependent velocity field $\vec{u} \in \otimes_{n=1}^{d}(\tilde{\mathscr{A}}_{\mathcal{T}} \otimes L^2(\mathcal{V}))$, as well as extending the result to $\boldsymbol{\kappa}^*$. The details are as follows.

Consider the Hilbert spaces $\mathcal{H}_{\mathcal{T}}$ and $\mathcal{H}_{\mathcal{V}}$ (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 $\mathcal{H}_{\mathcal{T}\mathcal{V}}$,

$$\mathcal{H}_{\mathcal{T}\mathcal{V}} = \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}_{\mathcal{V}}, \quad \mathcal{H}_{\mathcal{T}} = \{f \in L^2(\mathcal{V}) \mid f(0) = f(T)\}, \quad \mathcal{H}_{\mathcal{V}} = \{f \in L^2(\mathcal{V}) \mid f(0) = f(\vec{V})\}, \tag{42}$$

which are analogous to the Hilbert spaces $\mathscr{H}_{\mathcal{T}}$, $\mathscr{H}_{\mathcal{V}}$, and $\mathscr{H}_{\mathcal{T}\mathcal{V}}$ of vector-valued functions defined in equation (15). 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 $\langle f, h\rangle = \langle \overline{f}\, h\rangle$ 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 $\mathcal{H}_{\mathcal{T}\mathcal{V}}$-inner-product. Analogous to the Hilbert space $\mathscr{H}_{\times} \subset \mathscr{H}_{\mathcal{V}}$ defined in equation (16), we consider the Sobolev space $\mathcal{H}^1_{\mathcal{V}} \subset \mathcal{H}_{\mathcal{V}}$

$$\mathcal{H}^1_{\mathcal{V}} = \{f \in \mathcal{H}_{\mathcal{V}} \mid \langle|\vec{\nabla} f|^2\rangle_{\mathcal{V}} < \infty\}, \tag{43}$$

which is also a Hilbert space [11]. Here, $\langle\cdot\rangle_{\mathcal{V}}$ denotes spatial averaging over $\mathcal{V}$. Finally, consider the function space $\mathcal{F}$ with inner-product $\langle\cdot,\cdot\rangle_1$

$$\mathcal{F} = \{f \in \tilde{\mathscr{A}}_{\mathcal{T}} \otimes \mathcal{H}^1_{\mathcal{V}} \mid \langle f\rangle = 0\}, \qquad \langle f, g\rangle_1 = \left\langle \overline{\vec{\nabla} f} \cdot \vec{\nabla} g \right\rangle, \tag{44}$$

which is analogous to $\mathscr{F}$ in (22) and involves the space $\tilde{\mathscr{A}}_{\mathcal{T}}$ of absolutely continuous, $\mathcal{T}$–periodic, scalar-valued functions defined in equation (21). We denote by $\|\cdot\|_1$ the norm induced by the $\mathcal{F}$-inner-product, where $h \in \mathcal{F}$ implies that $\|\partial_t h\|_1 < \infty$ and $\|h\|_1 < \infty$. In the case of a time-independent velocity field $\vec{u}$ we set $\tilde{\mathscr{A}}_{\mathcal{T}} = \emptyset$ in (44), so that $h \in \mathcal{F}$ implies $h \in \mathcal{H}^1_{\mathcal{V}}$ with $\langle h\rangle_{\mathcal{V}} = 0$.

In terms of the $\mathcal{F}$-inner-product $\langle\cdot,\cdot\rangle_1$, the components κ^*_{jk} and α^*_{jk}, $j, k = 1, \ldots, d$, of the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ are given by the following functionals [29],

$$\kappa^*_{jk} = \varepsilon(\delta_{jk} + \langle\chi_j, \chi_k\rangle_1), \qquad \alpha^*_{jk} = \langle A\chi_j, \chi_k\rangle_1, \quad A = \Delta^{-1}(\vec{u}\cdot\vec{\nabla} - \partial_t), \tag{45}$$

which are analogous to that in (9). The formulas for κ^*_{jk} and α^*_{jk} in equation (45) follow [29] from $\mathcal{K}^*_{jk} = \varepsilon\delta_{jk} + \langle u_j\chi_k\rangle$ in (A-12) and the cell problem $-\varepsilon\Delta\chi_j - (\vec{u}\cdot\vec{\nabla} - \partial_t)\chi_j = u_j$ in equation (A-9):

$$\langle u_j\chi_k\rangle = \langle\Delta\Delta^{-1}u_j\chi_k\rangle = -\langle\vec{\nabla}\Delta^{-1}u_j\cdot\vec{\nabla}\chi_k\rangle = -\langle\Delta^{-1}u_j,\chi_k\rangle_1 = \varepsilon\langle\chi_j,\chi_k\rangle_1 + \langle A\chi_j,\chi_k\rangle_1, \tag{46}$$

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 (45), which is analogous to equation (27),

$$\chi_j = (\varepsilon + A)^{-1}g_j, \qquad g_j = (-\Delta)^{-1}u_j. \tag{47}$$

In equation (A-14) of Section A-1.3 we show that the incompressibility of $\vec{u}$ in (2) implies that the operator $(\Delta^{-1})(\vec{u}\cdot\vec{\nabla})$ is anti-symmetric on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$ [6]. Moreover, for $\vec{u}\in\otimes^d_{n=1}\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}_\mathcal{V}$, we also have that it is a bounded operator on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$. Indeed, since $\Delta = \vec{\nabla}\cdot\vec{\nabla}$, we have

$$\|(\Delta^{-1})h\|^2_1 = \langle\vec{\nabla}(\Delta^{-1})h\cdot\vec{\nabla}(\Delta^{-1})h\rangle = \langle[(-\Delta)^{-1}h]\,h\rangle, \quad \forall\, h\in\mathcal{F}, \tag{48}$$

which implies that

$$\|(\Delta^{-1})(\vec{u}\cdot\vec{\nabla})h\|^2_1 = |\langle[(\Delta^{-1})(\vec{u}\cdot\vec{\nabla})h]\,(\vec{u}\cdot\vec{\nabla})h\rangle| \le \|(\Delta^{-1})\|\,\|\vec{u}\|^2\|h\|^2_1 < \infty, \tag{49}$$

where we have used the simplified notation $\|\vec{u}\|^2 = \sum_j\|u_j\|^2$ and the fact [33] that (Δ^{-1}) is compact, hence bounded on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$. Since $(\Delta^{-1})(\vec{u}\cdot\vec{\nabla})$ is bounded anti-symmetric operator on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$, the operator $\imath(\Delta^{-1})(\vec{u}\cdot\vec{\nabla})$ is self-adjoint on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$. 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 $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$, which implies that $\imath(\Delta^{-1})\partial_t$ is self-adjoint on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$. It is now clear that $M = -\imath A$, with $A = (\Delta^{-1})(\vec{u}\cdot\vec{\nabla} - \partial_t)$ is self-adjoint on $\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}^1_\mathcal{V}$. Finally, since an operator is self-adjoint if and only if it is a maximal normal operator [34], we have that A is a maximal normal operator on the function space $\mathcal{F}$. Using this alternative Hilbert space formulation of the effective parameter problem for $\mathcal{K}^*$, we have the following corollary of Theorem 4.1.

Corollary 4.1. *Let $z = \imath\lambda$, $g_j = -(\Delta^{-1})u_j$ be defined as in (47), 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 (45), with domain $\mathcal{F}$ defined in (44). 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 $\mu_{kk}(\lambda) = \|Q_2(\lambda)g_k\|^2_1$. Moreover, consider the real-valued functions $\mathrm{Re}\,\mu_{jk}(\lambda)$ and $\mathrm{Im}\,\mu_{jk}(\lambda)$ defined in (34). 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 (35) hold for the functionals κ^*_{jk} and α^*_{jk} defined in equation (45). The domain of integration I is determined by the spectrum $\Sigma(A)$ of the operator A, where $I\subseteq[-\|A\|,\|A\|]$ and $\|A\|\le\|(\Delta^{-1})\|\|\vec{u}\|\|\vec{\nabla}\|_1<\infty$ in the case of a time-independent velocity field $\vec{u}$.*

Proof of Corollary 4.1. From equations (45) and (47) we have the following analogue of (36)

$$\kappa^*_{jk} = \varepsilon\left(\delta_{jk} + \langle(\varepsilon + A)^{-1}g_j, (\varepsilon + A)^{-1}g_k\rangle_1\right), \quad \alpha^*_{jk} = \langle A(\varepsilon + A)^{-1}g_j, (\varepsilon + A)^{-1}g_k\rangle_1, \tag{50}$$

where $g_j = -(\Delta^{-1})u_j$. By the proof of Theorem 4.1 and the properties $\chi_j, A\chi_j : \mathbb{R}\times\mathbb{R}^d\to\mathbb{R}$, we need only to prove that $g_j\in\mathcal{F}$ for all $j = 1,\ldots,d$. By equation (48) and $\vec{u}\in\otimes^d_{n=1}\tilde{\mathscr{A}_\mathcal{T}}\otimes\mathcal{H}_\mathcal{V}$, for each $t\in\mathcal{T}$ fixed, we have

$$\|g_j(t,\cdot)\|^2_1 = |\langle[(\Delta^{-1})u_j(t,\cdot)]\,u_j(t,\cdot)\rangle| \le \|(\Delta^{-1})\|\,\|u_j(t,\cdot)\|^2 < \infty, \tag{51}$$

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

$$\|\partial_t g_j(\cdot, \vec{x})\|_1 = \|\partial_t(\Delta^{-1})u_j(\cdot, \vec{x})\|_1 = \|(\Delta^{-1})\partial_t u_j(\cdot, \vec{x})\|_1 \leq \|\Delta^{-1}\| \, \|\partial_t u_j(\cdot, \vec{x})\|^2 < \infty. \tag{52}$$

Finally, from equation (2) we have that $\langle u_j(\cdot, \vec{x})\rangle = 0$ for each $\vec{x} \in \mathcal{V}$ fixed. Therefore, by Fubini's theorem [12] we have that $\langle g_j\rangle = 0$. Consequently, $g_j \in \mathcal{F}$ for all $j = 1, \ldots, d$, which establishes that the integral representations in equation (35) hold for the functionals κ^*_{jk} and α^*_{jk} defined in (45). Analogous to (37), by equation (48) the mass μ^0_{jk} of the associated measure $\mathrm{d}\mu_{jk}$ is given by

$$\mu^0_{jk} = \langle g_j, g_k\rangle_1 = \langle [(-\Delta)^{-1}u_j] \, u_k\rangle, \tag{53}$$

which implies that $|\mu^0_{jk}| \leq \|\Delta^{-1}\| \, \|u_j\| \, \|u_k\| < \infty$. The domain of integration I in (35) is determined by the spectrum $\Sigma(A)$ of the operator A, where $I \subseteq [-\|A\|, \|A\|]$ and $\|A\| \leq \|(\Delta^{-1})\|\|\vec{u}\|\|\vec{\nabla}\|_1 < \infty$ in the case of a time-independent velocity field $\vec{u}$. This concludes our proof of Corollary 4.1 $\square$.

4.3. **An isometric correspondence.** A natural question to ask is the following. Is the formulation of the effective parameter problem described in Theorem 2.1 equivalent to that described in Corollary 4.1? The correspondence between the two formulations is one of isometry, and is summarized by the following theorem.

Theorem 4.2. *The function spaces $\mathscr{F}$ and $\mathcal{F}$ defined in equations* (22) *and* (44) *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* (27) *and* (45)*, respectively. Specifically, for every $f \in D(A)$ we have $\vec{\nabla} f \in D(\mathbf{A})$ and $\|Af\|_1 = \|\mathbf{A}\vec{\nabla} f\|$, and conversely, for each $\vec{\xi} \in D(\mathbf{A})$ there exists unique $f \in D(A)$ such that $\vec{\xi} = \vec{\nabla} f$ and $\|\mathbf{A}\vec{\xi}\| = \|Af\|_1$. The Radon–Stieltjes measures underlying the integral representations of Theorem 2.1 and Corollary 4.1 are equal, $\mathrm{d}\langle Q_2(\lambda)g_j, g_k\rangle_1 = \mathrm{d}\langle \mathbf{Q}_2(\lambda)\vec{g}_j, \vec{g}_k\rangle$, $j, k = 1, \ldots, d$, up to null sets of measure zero, where $\vec{g}_j = \vec{\nabla} g_j$. Moreover, the operators $\mathbf{A}$ and A are related by $\mathbf{A}\vec{\nabla} = \vec{\nabla} A$, which implies and is implied by the weak equality $\mathbf{Q}_2(\lambda)\vec{\nabla} = \vec{\nabla} Q_2(\lambda)$.*

Proof of Theorem 4.2. We use the formula $\vec{u} = \vec{\nabla} \cdot \mathbf{H}$ displayed in equation (3) to write the operator $A = \Delta^{-1}(\vec{u} \cdot \vec{\nabla} - \partial_t)$ and function $g_j = (-\Delta)^{-1}u_j$ defined in equations (45) and (47) as $A = \Delta^{-1}(\vec{\nabla} \cdot \mathbf{H}\vec{\nabla} - \partial_t)$ and $g_j = (-\Delta)^{-1}\vec{\nabla} \cdot \mathbf{H}\vec{e}_j$, respectively. Using the definition $\mathbf{\Gamma} = \vec{\nabla}(\Delta^{-1})\vec{\nabla}\cdot$ and the formulas $\vec{\nabla}\Delta^{-1}\partial_t = \mathbf{\Delta}^{-1}\mathbf{T}\vec{\nabla}$, $\vec{g}_j = -\mathbf{\Gamma}\mathbf{H}\vec{e}_j$, and $\mathbf{A} = \mathbf{\Gamma}\mathbf{H} - \mathbf{\Delta}^{-1}\mathbf{T}$ displayed in equations (11), (27), and (28), respectively, we have that

$$\vec{\nabla} A = [\mathbf{\Gamma}\mathbf{H} - \mathbf{\Delta}^{-1}\mathbf{T}]\vec{\nabla} = \mathbf{A}\vec{\nabla}, \qquad \vec{\nabla} g_j = \vec{g}_j. \tag{54}$$

Consequently, by applying the differential operator $\vec{\nabla}$ to both sides of the formula $(\varepsilon + A)\chi_j = g_j$ of (47), we obtain the formula $(\varepsilon\mathbf{I} + \mathbf{A})\vec{\nabla}\chi_j = \vec{g}_j$ of equation (27).

Since the function spaces $\mathcal{F}$ and $\mathscr{F}$ differ only in the characterization of the spatial variable $\vec{x}$, we now discuss the relationship between the Hilbert spaces $\mathscr{H}_\times$ and $\mathcal{H}^1_\mathcal{V}$ defined in equations (16) and (43), respectively, with inner-product induced norms $\|\cdot\|$ and $\|\cdot\|_1$. For $f \in \mathcal{H}^1_\mathcal{V} \subset L^2(\mathcal{V})$ we have $\Delta^{-1}\Delta f = f$ [33], which implies that $\mathbf{\Gamma}\vec{\nabla} f = \vec{\nabla} f$ and $\|\vec{\nabla} f\|^2 = \langle \vec{\nabla} f \cdot \vec{\nabla} f\rangle = \|f\|^2_1 < \infty$. Consequently, for every $f \in \mathcal{H}^1_\mathcal{V}$ we have $\vec{\nabla} f \in \mathscr{H}_\times$. Conversely, $\vec{\xi} \in \mathscr{H}_\times$ implies that $\vec{\xi} = \mathbf{\Gamma}\vec{\xi} = \vec{\nabla} f$, where we have defined the scalar-valued function $f = \Delta^{-1}\vec{\nabla} \cdot \vec{\xi}$. Since $\vec{\xi} = \vec{\nabla} f$, the $\mathcal{H}^1_\mathcal{V}$ norm of f satisfies $\|f\|^2_1 = \langle \vec{\xi} \cdot \vec{\xi}\rangle = \|\vec{\xi}\|^2 < \infty$ so that $f \in \mathcal{H}^1_\mathcal{V}$. Moreover, f is uniquely determined by $\vec{\xi}$ up to equivalence class, since if $f_1 = \Delta^{-1}\vec{\nabla} \cdot \vec{\xi}$ and $f_2 = \Delta^{-1}\vec{\nabla} \cdot \vec{\xi}$ then $\mathbf{\Gamma}\vec{\xi} = \vec{\xi}$ implies that $\|f_1 - f_2\|_1 = \|\vec{\xi} - \vec{\xi}\| = 0$. Consequently, for every $\vec{\xi} \in \mathscr{H}_\times$ there exists unique $f \in \mathcal{H}^1_\mathcal{V}$ such that $\vec{\xi} = \vec{\nabla} f$. In summary, the Hilbert spaces $\mathcal{H}^1_\mathcal{V}$ and $\mathscr{H}_\times$ are in one-to-one isometric correspondence, which we denote by $\mathcal{H}^1_\mathcal{V} \sim \mathscr{H}_\times$. This, in turn, implies that $\mathcal{F} \sim \mathscr{F}$.

We now return to our previous notation, where $\|\cdot\|_1$ and $\|\cdot\|$ denotes the norm induced by the $\mathcal{F}$- and $\mathscr{F}$-inner-product, respectively. We demonstrate that the one-to-one isometry between $\mathcal{F}$ and $\mathscr{F}$ induces a one-to-one isometry between the domains $D(A)$ and $D(\mathbf{A})$ of the operators A and $\mathbf{A}$, i.e. $D(A)\sim D(\mathbf{A})$. This, in turn, follows from another on-to-one isometry between the class of self-adjoint operators on $\mathcal{F}$, for example, and the class of resolutions of the identity. This correspondence is determined directly as follows [34]. Let X be a self-adjoint operator on $\mathcal{F}$ and $Q(\lambda)$ be the associated resolution of the identity, which is a one-to-one correspondence [34]. The domain $D(X)$ of X comprises those and only those elements $f\in\mathcal{F}$ such that the Stieltjes integral $\int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}\|Q(\lambda)f\|_1^2$ is convergent; when $f\in D(X)$ the element Xf is determined by the relations

$$\langle Xf,h\rangle_1=\int_{-\infty}^{\infty}\lambda\,\mathrm{d}\langle Q(\lambda)f,h\rangle_1,\qquad \|Xf\|_1^2=\int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}\|Q(\lambda)f\|_1^2, \tag{55}$$

where h is an arbitrary element in $\mathcal{F}$ [34]. Since $M=-\imath A$ is self-adjoint on $\mathcal{F}$ and $D(A)=D(M)$, this one-to-one isometric correspondence also holds for the maximal normal operator A, and a calculation similar to that in equations (40) and (41) shows that equation (55) 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 $\mathscr{F}$ with $D(\mathbf{A})=D(\mathbf{M})$.

We now demonstrate that the one-to-one isometry between the class of self-adjoint operators and resolutions of the identity on $\mathcal{F}$, and that for $\mathscr{F}$, along with the property $\mathcal{F}\sim\mathscr{F}$ and equation (54), induce the one-to-one isometry $D(A)\sim D(\mathbf{A})$. From $\mathcal{F}\sim\mathscr{F}$, we have for every $f\in D(A)\subset\mathcal{F}$ that $\vec{\nabla}f\in\mathscr{F}$, so from equation (54)

$$\|Af\|_1^2=\langle Af,Af\rangle_1=\langle\vec{\nabla}Af\cdot\vec{\nabla}Af\rangle=\langle\mathbf{A}\vec{\nabla}f\cdot\mathbf{A}\vec{\nabla}f\rangle=\|\mathbf{A}\vec{\nabla}f\|^2. \tag{56}$$

Consequently, from equation (55) we have

$$\int\lambda^2\,\mathrm{d}\|Q_2(\lambda)f\|_1^2=\int\lambda^2\,\mathrm{d}\|\mathbf{Q}_2(\lambda)\vec{\nabla}f\|^2, \tag{57}$$

and the convergence of the left-hand-side of (57) implies the convergence of the right-hand-side which, in turn, implies that $\vec{\nabla}f\in D(\mathbf{A})$. Conversely, from $\mathcal{F}\sim\mathscr{F}$ we have that $\vec{\xi}\in D(\mathbf{A})\subset\mathscr{F}$ implies there exists unique $f\in\mathcal{F}$ such that $\vec{\xi}=\vec{\nabla}f$, and equation (54) then implies that

$$\|\mathbf{A}\vec{\xi}\|^2=\langle\mathbf{A}\vec{\nabla}f,\mathbf{A}\vec{\nabla}f\rangle=\langle\vec{\nabla}Af,\vec{\nabla}Af\rangle=\langle Af,Af\rangle_1=\|Af\|_1^2. \tag{58}$$

Again, equation (55) implies that (57) holds, and the convergence of the right-hand-side of (57) 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 $\vec{\nabla}f\in D(\mathbf{A})$ and $\|Af\|_1^2=\|\mathbf{A}\vec{\nabla}f\|^2$. Conversely, for each $\vec{\xi}\in D(\mathbf{A})$ there exists unique $f\in D(A)$ such that $\vec{\xi}=\vec{\nabla}f$ and $\|\mathbf{A}\vec{\xi}\|^2=\|Af\|_1^2$. 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 $\vec{\nabla}Q_2(\lambda)=\mathbf{Q}_2(\lambda)\vec{\nabla}$, 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 (57) and the linearity properties of Radon–Stieltjes integrals [34], we have that

$$0=\int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}(\|Q_2(\lambda)f\|_1^2-\|\mathbf{Q}_2(\lambda)\vec{\nabla}f\|^2)=\int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}(\langle[\vec{\nabla}Q_2(\lambda)-\mathbf{Q}_2(\lambda)\vec{\nabla}]f\cdot\vec{\nabla}f\rangle). \tag{59}$$

Equation (59) implies that for all $f\in D(A)\iff\vec{\nabla}f\in D(\mathbf{A})$ we have $\mathrm{d}\|Q_2(\lambda)f\|_1^2=\mathrm{d}\|\mathbf{Q}_2(\lambda)\vec{\nabla}f\|^2$, up to null sets of measure zero. Moreover, the equality $\vec{\nabla}Q_2(\lambda)=\mathbf{Q}_2(\lambda)\vec{\nabla}$ holds weakly. Conversely, assume that $Q_2(\lambda)$ and $\mathbf{Q}_2(\lambda)$ are the resolutions of the identity associated with the operators A and $\mathbf{A}$ on the function spaces $\mathcal{F}$ and $\mathscr{F}$, respectively, which is a one-to-one correspondence [34], and that $\vec{\nabla}Q_2(\lambda)f=\mathbf{Q}_2(\lambda)\vec{\nabla}f$ holds for every $f\in D(A)\iff\vec{\nabla}f\in D(\mathbf{A})$. Then equation (59) holds and implies equation (57). The correspondence $D(A)\sim D(\mathbf{A})$ and equation (55) then imply that

$\|\mathbf{A}\vec{\nabla}f\|^2 = \|Af\|_1^2 = \|\vec{\nabla}Af\|^2$, hence $\|(\mathbf{A}\vec{\nabla} - \vec{\nabla}A)f\|^2 = 0$ for every $f \in D(A) \iff \vec{\nabla}f \in D(\mathbf{A})$, which implies that $\mathbf{A}\vec{\nabla} = \vec{\nabla}A$ weakly. Since $g_k \in D(A)$ and $\vec{g}_k \in D(\mathbf{A})$ with $\vec{g}_k = \vec{\nabla}g_k$, this result implies that the Radon–Stieltjes measures underlying the integral representations of Theorem 2.1 and Corollary 4.1 are equal $\mathrm{d}\langle Q_2(\lambda)g_j, g_k\rangle_1 = \mathrm{d}\langle \mathbf{Q}_2(\lambda)\vec{g}_j, \vec{g}_k\rangle$ up to null sets of measure zero, for all $j, k = 1, \dots, d$. This concludes our proof of Theorem 4.2 □.

4.4. **Discrete integral representations by eigenfunction expansion.** The integral representations of Theorem 4.1 and Corollary 4.1 for κ^*_{jk} and α^*_{jk}, displayed in equation (35), involve spectral measures $\mathrm{d}\mu_{jk}(\lambda)$, $j, k = 1, \dots, d$, which have discrete and continuous components [31, 34]. 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 5, which exploits Fourier methods to calculate κ^*_{jk} and α^*_{jk} for a large class of velocity fields. This, in turn, provides numerical methods for the computation of κ^*_{jk} and α^*_{jk} for such velocity fields, which will be exploited in Section 7.

We now summarize some general spectral properties of the maximal, anti-symmetric operators $\mathbf{A}$ and A on the function spaces $\mathscr{F}$ and $\mathcal{F}$ defined in equations (22) and (44), respectively, which are dense subsets of their associated Hilbert spaces $\mathscr{H}^\times$ and $\mathcal{H}^1$,

$$\mathscr{H}^\times = \{\vec{\xi} \in \mathscr{H}_{\mathcal{T}} \otimes \mathscr{H}_\times \mid \langle\vec{\xi}\rangle = 0\}, \quad \mathcal{H}^1 = \{f \in \mathcal{H}_{\mathcal{T}} \otimes \mathcal{H}^1_{\mathcal{V}} \mid \langle f\rangle = 0\}. \tag{60}$$

See equations (15) and (42) for the notational definitions of equation (60). For simplicity, we focus on the opertor A and the Hilbert space $\mathcal{H}^1$, as the discussion regarding $\mathbf{A}$ and $\mathscr{H}^\times$ is analogous.

Recall that the domain $D(A)$ of the maximal normal operator A comprises those and only those elements $f \in \mathcal{F}$ such that $\|Af\|_1^2 = \int_{-\infty}^{\infty} \lambda^2\, \mathrm{d}\|Q(\lambda)f\|_1^2 < \infty$, where $Q(\lambda)$ is the projection valued operator corresponding to A [34]. The integration is over the spectrum $\Sigma(A)$ of A, which has continuous Σ_{cont} and discrete (pure-point) Σ_{pp} components, $\Sigma(A) = \Sigma_{\text{cont}}(A) \cup \Sigma_{\text{pp}}(A)$. We first focus on the discrete spectrum $\Sigma_{\text{pp}}(A)$. The members $f \neq 0$ of $D(A)$ which satisfy $Af = \upsilon f$ with $\upsilon \in \Sigma_{\text{pp}}(A)$ are called eigenfunctions and υ is the corresponding eigenvalue. The span of all eigenfunctions is a *countable* subspace of $D(A)$ [31, 34]. Accordingly, we will denote the eigenfunctions by φ_n, $n = 1, 2, \dots$, with corresponding eigenvalues υ_n. Since A is anti-symmetric, υ_n is purely imaginary [34, 17] 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 [34], i.e. if $A\varphi_n = \upsilon_n\varphi_n$, $A\varphi_m = \upsilon_m\varphi_m$, and $\upsilon_n \neq \upsilon_m$, then

$$\langle \varphi_n, \varphi_m\rangle_1 = \langle \vec{\nabla}\varphi_n \cdot \vec{\nabla}\varphi_m\rangle = \delta_{nm}. \tag{61}$$

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 [34]. 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 $\mathcal{H}^1$.

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

Theorem 4.3 ([34] pages 189 and 247)**.** *One of the three cases must occur:*

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

manifolds $\mathcal{M}(\varphi_n)$ and $\mathcal{N}(\psi_m)$ are mutually orthogonal and together determine $\mathcal{H}^1$ according to

$$\mathcal{M} = \oplus_{n=1}^{\infty}\mathcal{M}_n(\varphi_n), \qquad \mathcal{N} = \oplus_{m=1}^{\infty}\mathcal{N}_m(\psi_m), \qquad \mathcal{H}^1 = \mathcal{M}\oplus\mathcal{N}$$

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

In each of the three cases, the closed linear manifolds $\mathcal{M}$ and $\mathcal{N}$ reduce A [34].

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

Theorem 4.4. *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 [34]

$$\|A\varphi_n\|_1^2 = \int_{-\infty}^{\infty}\lambda^2\,\mathrm{d}\|Q(\lambda)\varphi_n\|_1^2 = \lambda_n^2, \qquad \langle A\varphi_n, h\rangle_1 = \int_{-\infty}^{\infty}\lambda\,\mathrm{d}\langle Q(\lambda)\varphi_n, h\rangle_1 = \lambda_n\langle\varphi_n, h\rangle_1, \tag{62}$$

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 4.3 is that

$$f = \sum_{n=1}^{\infty} a_n\varphi_n, \quad a_n = \langle f, \varphi_n\rangle_1, \quad \|f\|_1^2 = \sum_{n=1}^{\infty}|a_n|^2 \neq 0. \tag{63}$$

Furthermore, for such an element f we have

$$\|Q(\lambda)f\|_1^2 = \sum_{n:\,\lambda_n\leq\lambda}|a_n|^2, \quad A\varphi_n = \imath\lambda_n\varphi_n. \tag{64}$$

A characterization of continuous spectrum Σ_{cont} in terms of $Q(\lambda)$ and $\mathcal{N}$ is the following. A necessary and sufficient condition that $f \neq 0$ be an element of $\mathcal{N}$ is that $\|Q(\lambda)f\|_1^2$ be a continuous function of λ not identically zero. The following theorem is a refinement of cases (1) and (2) of Theorem 4.3.

Theorem 4.5 ([34] page 250)**.** *The orthonormal set $\{\psi_m\}$ of Theorem 4.3 can be replaced by an orthonormal set $\{\phi_m\}$ such that*

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

$$\varrho_{k+1}(\lambda) = \int_{-\infty}^{\lambda}F(\xi)\mathrm{d}\varrho_k(\xi), \qquad \varrho_k(\lambda) = \|Q(\lambda)\phi_k\|_1^2, \qquad F(\lambda) = \frac{\mathrm{d}\varrho_{k+1}}{\mathrm{d}\varrho_k}, \tag{65}$$

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

The following theorem [34] provides an explicit representation for the standard decomposition of the Stieltjes measure $\mathrm{d}\mu(\lambda)$ into its continuous and discrete components.

Theorem 4.6 ([34] 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*

$$\|Q(\lambda)f\|_1^2 = \|Q(\lambda)g\|_1^2 + \|Q(\lambda)h\|_1^2, \qquad \mathrm{d}\|Q(\lambda)f\|_1^2 = \mathrm{d}\|Q(\lambda)g\|_1^2 + \mathrm{d}\|Q(\lambda)h\|_1^2 \tag{66}$$

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 [31] $\mathcal{N} = \mathcal{N}_{\mathrm{ac}} \otimes \mathcal{N}_{\mathrm{sing}}$, with $h = h_{\mathrm{ac}} + h_{\mathrm{sing}}$, to provide the standard [12] 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,

$$\mathrm{d}\|Q(\lambda)h\|_1^2 = \mathrm{d}\|Q(\lambda)h_{\mathrm{ac}}\|_1^2 + \mathrm{d}\|Q(\lambda)h_{\mathrm{sing}}\|_1^2. \tag{67}$$

However, the sets $\mathcal{N}_{\mathrm{ac}}$ and $\mathcal{N}_{\mathrm{sing}}$ need not be disjoint [31].

We now use the mathematical framework summarized above to provide explicit formulas for the discrete component of the integral representations for κ^*_{jk} and α^*_{jk}, displayed in equation (35). For simplicity, we focus on the formulation of the effective parameter problem described by Corollary 4.1, as that of Theorem 4.1 is analogous. Recall the cell problem of equations (47) and (A-9), written as

$$(\varepsilon + A)\chi_j = g_j, \quad g_j = (-\Delta)^{-1}u_j, \tag{68}$$

where A is defined in equation (45) and u_j, $j = 1,\dots,d$, is the j^{th} component of the velocity field $\vec{u}$. Since $\chi_j, g_j \in \mathcal{F} \subset \mathcal{H}^1$, by the formula $\mathcal{H}^1 = \mathcal{M} \oplus \mathcal{N}$ of Theorem 4.3 and equation (63), they have the following representations

$$\chi_j = \sum_n \langle\varphi_n, \chi_j\rangle_1\, \varphi_n + \chi_j^\perp, \qquad g_j = \sum_n \langle\varphi_n, g_j\rangle_1\, \varphi_n + g_j^\perp, \tag{69}$$

where $\varphi_n \in \mathcal{M}$ and $\chi_j^\perp, g_j^\perp \in \mathcal{N}$. Inserting (69) into the cell problem (68) and using $A\varphi_n = \imath\lambda_n\varphi_n$ yields

$$\sum_n [(\varepsilon + \imath\lambda_n)\langle\varphi_n, \chi_j\rangle_1 - \langle\varphi_n, g_j\rangle_1]\varphi_n + (\varepsilon + A)\chi_j^\perp - g_j^\perp = 0. \tag{70}$$

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 (70) with φ_n yields

$$\langle\varphi_n, \chi_j\rangle_1 = \frac{\langle\varphi_n, g_j\rangle_1}{(\varepsilon + \imath\lambda_n)}, \quad 0 < \varepsilon < \infty. \tag{71}$$

Recall the representations $\kappa^*_{jk} = \varepsilon(\delta_{jk} + \langle\chi_j, \chi_k\rangle_1)$ and $\alpha^*_{jk} = \langle A\chi_j, \chi_k\rangle_1$, $j, k = 1,\dots,d$, displayed in equation (45). From equations (69) and (71), the orthonormality of the set $\{\varphi_n\}$, and the mutual orthogonality of $\mathcal{M}$ and $\mathcal{N}$, we have

$$\begin{aligned} \langle\chi_j, \chi_k\rangle_1 - \langle\chi_j^\perp, \chi_k^\perp\rangle_1 &= \sum_n \overline{\langle\varphi_n, \chi_j\rangle}_1\langle\varphi_n, \chi_k\rangle_1 = \sum_n \frac{\overline{\langle\varphi_n, g_j\rangle}_1\langle\varphi_n, g_k\rangle_1}{\varepsilon^2 + \lambda_n^2} \\ \langle A\chi_j, \chi_k\rangle_1 - \langle A\chi_j^\perp, \chi_k^\perp\rangle_1 &= \sum_n -\imath\lambda_n\, \overline{\langle\varphi_n, \chi_j\rangle}_1\langle\varphi_n, \chi_k\rangle_1 = \sum_n \frac{-\imath\lambda_n\, \overline{\langle\varphi_n, g_j\rangle}_1\langle\varphi_n, g_k\rangle_1}{\varepsilon^2 + \lambda_n^2}. \end{aligned} \tag{72}$$

The right hand sides of the formulas in equation (72) 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 [34].

A direct correspondence can be made between the integrals in equations (72) and (35) 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

$$\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1=\langle g_j|\,|\varphi_n\rangle\overline{\langle\varphi_n|}\,|g_j\rangle=\langle g_j|Q_n|g_k\rangle, \tag{73}$$

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

$$\mathrm{d}\mu_{jk}(\lambda)=\langle g_j|Q(\lambda)|g_k\rangle\,\delta_{\lambda_n}(\mathrm{d}\lambda),\qquad Q(\lambda)=\sum_{n\colon\lambda_n\leq\lambda}Q_n,\quad Q_n=|\varphi_n\rangle\overline{\langle\varphi_n|},\quad \lambda\in\Sigma_{\mathrm{pp}}(A), \tag{74}$$

where $\delta_{\lambda_n}(\mathrm{d}\lambda)$ is the delta measure concentrated at λ_n. Moreover, exactly as in equations (39) and (41), we may use the fact that the function g_j and molecular diffusivity ε are real-valued, to re-express the integrals in (72), 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

$$\begin{aligned}\mathrm{dRe}\,\mu_{jk}(\lambda)&=\mathrm{Re}\langle g_j|Q(\lambda)|g_k\rangle\,\delta_{\lambda_n}(\mathrm{d}\lambda),\qquad \mathrm{Re}\langle g_j|Q(\lambda)|g_k\rangle=\sum_{n\colon\lambda_n\leq\lambda}\mathrm{Re}[\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1]\\ \mathrm{dIm}\,\mu_{jk}(\lambda)&=\mathrm{Im}\langle g_j|Q(\lambda)|g_k\rangle\,\delta_{\lambda_n}(\mathrm{d}\lambda),\qquad \mathrm{Im}\langle g_j|Q(\lambda)|g_k\rangle=\sum_{n\colon\lambda_n\leq\lambda}\mathrm{Im}[\overline{\langle\varphi_n,g_j\rangle}_1\langle\varphi_n,g_k\rangle_1].\end{aligned} \tag{75}$$

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 $u_j(t,\cdot)\in\mathcal{H}^1(\mathcal{V})\subset L^2(\mathcal{V})$ we have [33]

$$\langle\varphi_n,g_j\rangle_1=\langle\vec\nabla\varphi_n\cdot\vec\nabla(-\Delta)^{-1}u_j\rangle=\langle\varphi_n,(-\Delta)(-\Delta)^{-1}u_j\rangle_2=\langle\varphi_n,u_j\rangle_2, \tag{76}$$

where $\langle\cdot,\cdot\rangle_2$ denotes the $L^2(\mathcal{T}\times\mathcal{V})$ inner-product. This property will be used in Section 5 to calculate κ^*_{jk} and α^*_{jk} for a large class of velocity fields.

4.5. **Finite dimensional matrix setting - curl free.** In this section, we demonstrate how the integral formulas of Theorem 2.1 and Corollary 4.1, displayed in equation (35), arise when the underlying operator is given by a matrix. This matrix formulation is useful when considering discrete approximations of the underlying operators. Such approximations will be considered in Section 7 to directly compute the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ for model velocity fields $\vec u$. Since the formulations of Theorem 2.1 and Corollary 4.1 involve a different inner-products, we must treat the two cases separately. We first consider the matrix formulation of Theorem 2.1 which involves the operator $\mathbf{A}=\mathbf{\Gamma S\Gamma}$ defined in equation (27), where $\mathbf{\Gamma}=\vec\nabla(-\Delta)^{-1}\vec\nabla\cdot$ and $\mathbf{S}=\mathbf{H}-(\mathbf{\Delta}^{-1})\mathbf{T}$ is defined in equation (9).

In this matrix setting, the differential operators ∂_t and $\vec\nabla$ are replaced by finite difference matrices $\mathbf{D}_t$ and $\boldsymbol{\nabla}$, respectively, where $\boldsymbol{\nabla}^T=(\mathbf{D}_1^T,\ldots,\mathbf{D}_d^T)$ and $\mathbf{D}_j$, $j=1,\ldots,d$, are also finite difference matrices. Consequently, the differential operators underlying the operator $\mathbf{A}$ are mapped to matrices as follows: $\mathbf{T}\mapsto\mathrm{diag}(\mathbf{D}_t,\ldots,\mathbf{D}_t)$, $\vec\nabla\mapsto\boldsymbol{\nabla}$, $\vec\nabla\cdot\mapsto\boldsymbol{\nabla}^T$, $\Delta\mapsto\boldsymbol{\nabla}^T\boldsymbol{\nabla}$, $\mathbf{\Delta}\mapsto\mathrm{diag}(\boldsymbol{\nabla}^T\boldsymbol{\nabla},\ldots,\boldsymbol{\nabla}^T\boldsymbol{\nabla})$. The inversions $(-\Delta)^{-1}$ and $\mathbf{\Delta}^{-1}$ are interpreted in terms of matrix inverse. Furthermore, in this matrix setting, $\mathbf{H}$ is a banded anti-symmetric matrix and $\mathbf{\Gamma}$ is a projection matrix which satisfies $\mathbf{\Gamma}^2=\mathbf{\Gamma}$. In this way, the integro-differential operator $\mathbf{A}$ is represented by an anti-symmetric matrix, $\mathbf{A}^T=-\mathbf{A}$, of size N, say, which we also denote by $\mathbf{A}$ for notational convenience. In a similar way, the vectors $\vec g_j$, $j=1,\ldots,d$, are redefined in this matrix setting.

The spectrum $\Sigma(\mathbf{A})$ of the matrix $\mathbf{A}$ consists solely of eigenvalues υ_n, $n\in I_N=\{1,\ldots,N\}$, i.e. $\Sigma(\mathbf{A})=\Sigma_{\mathrm{pp}}(\mathbf{A})=\{\upsilon_n\}$, with corresponding eigenvectors $\vec w_n$, $\mathbf{A}\vec w_n=\upsilon_n\vec w_n$. It is well known [17] that the eigenvalues υ_n are purely imaginary, $\upsilon_n=\imath\lambda_n$ with $\lambda_n\in\mathbb{R}$, and that the set of eigenvectors $\{\vec w_n\}_{n\in I_N}$ form an orthonormal basis [19] for $\mathbb{C}^N$, $\vec w_n\cdot\vec w_m=\vec w_n^\dagger\vec w_m=\delta_{nm}$, where † denotes the operation of complex-conjugate-transpose. Moreover, as $\mathbf{A}$ is real-valued, the eigenvalues υ_n and eigenvectors $\vec{w}_n$ come in complex-conjugate pairs [17]. Therefore, if the size N of the matrix $\mathbf{A}$ is even, then we may re-number the index set as $I_N = \{-N/2,\ldots,-1,1,\ldots,N/2\}$ such that $\upsilon_{-n} = \overline{\upsilon_n} = -\upsilon_n$ and $\vec{w}_{-n} = \overline{\vec{w}_n}$, and if N is odd then $\upsilon_0 = 0$ is also an eigenvalue with a *real-valued* eigenvector $\vec{w}_0$. Consequently, denoting by $\mathbf{W}$ the matrix with columns consisting of the eigenvectors $\vec{w}_n$, $\boldsymbol{\Upsilon} = \mathrm{diag}(\upsilon_{-N/2},\ldots,\upsilon_{N/2})$ the diagonal matrix with eigenvalues υ_n on the main diagonal, and $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_{-N/2},\ldots,\lambda_{N/2})$, we have $\mathbf{A} = \mathbf{W}\boldsymbol{\Upsilon}\mathbf{W}^\dagger = \imath\mathbf{W}\boldsymbol{\Lambda}\mathbf{W}^\dagger$. Here, the matrix $\mathbf{W}$ is unitary $\mathbf{W}^\dagger\mathbf{W} = \mathbf{W}\mathbf{W}^\dagger = \mathbf{I}$ so that the matrix $\mathbf{M} = -\imath\mathbf{A} = \mathbf{W}\boldsymbol{\Lambda}\mathbf{W}^\dagger$ is Hermitian [17, 19].

This spectral characterization of the matrix $\mathbf{A}$ leads to integral representations for κ^*_{jk} and α^*_{jk}, as defined by the functionals in equation (36). Since υ_n is purely imaginary and $0 < \varepsilon < \infty$, the matrix $(\varepsilon\mathbf{I}+\mathbf{A})$ has a well defined inverse given by $(\varepsilon\mathbf{I}+\mathbf{A})^{-1} = \mathbf{W}(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{W}^\dagger$ [17]. Therefore, since the (Hilbert space) adjoint of $\mathbf{W}$ is given by $\mathbf{W}^\dagger = \mathbf{W}^{-1}$ [17, 19], we have

$$\begin{aligned}\kappa^*_{jk}/\varepsilon - \delta_{jk} &= \langle(\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_j\cdot(\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_k\rangle = \langle(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{W}^\dagger\vec{g}_j\cdot(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{W}^\dagger\vec{g}_k\rangle,\\ \alpha^*_{jk} &= \langle\mathbf{A}(\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_j\cdot(\varepsilon\mathbf{I}+\mathbf{A})^{-1}\vec{g}_k\rangle = \langle\imath\boldsymbol{\Lambda}(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{W}^\dagger\vec{g}_j\cdot(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{W}^\dagger\vec{g}_k\rangle.\end{aligned}\tag{77}$$

A straightforward calculation shows that the functionals in equation (77) have the following discrete integral representations, which are analogous to those in equation (72),

$$\kappa^*_{jk}/\varepsilon - \delta_{jk} = \sum_{n\in I_N}\left\langle\frac{\overline{(\vec{w}_n^\dagger\vec{g}_j)}(\vec{w}_n^\dagger\vec{g}_k)}{\varepsilon^2+\lambda_n^2}\right\rangle,\qquad \alpha^*_{jk} = \sum_{n\in I_N}\left\langle\frac{-\imath\lambda_n\,\overline{(\vec{w}_n^\dagger\vec{g}_j)}(\vec{w}_n^\dagger\vec{g}_k)}{\varepsilon^2+\lambda_n^2}\right\rangle.\tag{78}$$

The spectral weights of these integrals are analogous to those in equation (73)

$$\overline{(\vec{w}_n^\dagger\vec{g}_j)}(\vec{w}_n^\dagger\vec{g}_k) = \vec{g}_j^{\,T}\,\vec{w}_n\vec{w}_n^\dagger\,\vec{g}_k = \vec{g}_j^{\,T}\mathbf{Q}_n\vec{g}_k = \mathbf{Q}_n\vec{g}_j\cdot\vec{g}_k\qquad \mathbf{Q}_n = \vec{w}_n\vec{w}_n^\dagger.\tag{79}$$

Here, $\mathbf{Q}_n = \vec{w}_n\vec{w}_n^\dagger$, $n\in I_N$, are mutually orthogonal, $\mathbf{Q}_n\mathbf{Q}_m = \mathbf{Q}_n\delta_{nm}$, Hermitian projection matrices onto the eigen-space spanned by the eigenvector $\vec{w}_n$. More specifically, since $\{\vec{w}_n\}$ is an orthonormal basis for $\mathbb{C}^N$, we have for all $\vec{\xi}\in\mathbb{C}^N$

$$\vec{\xi} = \sum_{n=1}^N(\vec{w}_n^\dagger\vec{\xi})\vec{w}_n = \sum_{n=1}^N(\vec{w}_n\vec{w}_n^\dagger)\vec{\xi} = \sum_{n=1}^N\mathbf{Q}_n\vec{\xi},\tag{80}$$

which implies the following resolution of the identity formula

$$\mathbf{I} = \sum_{n=1}^N\mathbf{Q}_n.\tag{81}$$

This implies that $\mathbf{A} = \sum_{n=1}^N\upsilon_n\mathbf{Q}_n$ and then $F(\mathbf{A}) = \sum_{n=1}^N F(\upsilon_n)\mathbf{Q}_n$ for all finite order polynomials $F(\upsilon)$. The following functional forms of this formula yield the matrix form of the spectral theorem displayed in equation (33),

$$[F(\mathbf{A})\vec{\xi}\cdot\vec{\zeta}\,] = \sum_{n=1}^N\overline{F(\upsilon_n)}[\mathbf{Q}_n\vec{\xi}\cdot\vec{\zeta}\,],\qquad [F(\mathbf{A})\vec{\xi}\cdot G(\mathbf{A})\vec{\zeta}\,] = \sum_{n=1}^N\overline{F(\upsilon_n)}G(\upsilon_n)[\mathbf{Q}_n\vec{\xi}\cdot\vec{\zeta}\,],\quad\forall\,\vec{\xi},\vec{\zeta}\in\mathbb{C}^N,\tag{82}$$

where $G(\upsilon)$ is also a finite order polynomial. Equation (78) is an extension of these formulas for functions of the form $F(\upsilon) = (\varepsilon+\upsilon)^{-1}$, and is immediately extendable to functions of the form $F(\upsilon) = (\varepsilon+\upsilon)^{-k}$ for arbitrary $k\in\mathbb{N}$, $0<\varepsilon<\infty$.

Analogous to equation (75), the spectral measure $\mathrm{d}\mu_{jk}(\lambda)$ and projection valued operator $\mathbf{Q}(\lambda)$ associated with equation (82) with $\vec{\xi} = \vec{g}_j$ and $\vec{\zeta} = \vec{g}_k$, and equation (78) are given by

$$\mathrm{d}\mu_{jk}(\lambda) = \langle[\mathbf{Q}(\lambda)\vec{g}_j\cdot\vec{g}_k\,]\,\delta_{\lambda_n}(\mathrm{d}\lambda)\rangle,\qquad \mathbf{Q}(\lambda) = \sum_{n:\,\lambda_n\le\lambda}\mathbf{Q}_n,\quad \mathbf{Q}_n = \vec{w}_n\vec{w}_n^\dagger.\tag{83}$$

Denoting an empty sum in (83) by the null matrix $\mathbf{0}$, the projection valued operator in (83) satisfies $\lim_{\lambda\to-\infty}\mathbf{Q}(\lambda)=\mathbf{0}$, and from (81) $\lim_{\lambda\to+\infty}\mathbf{Q}(\lambda)=\mathbf{I}$. With this notation, the discrete integral representations for κ^*_{jk} and α^*_{jk} displayed in (78) are direct analogues of that in equation (35). More specifically, exactly as in equations (39) and (41), we may use the fact that the matrix $\mathbf{A}$, vector $\vec{g}_j$, and molecular diffusivity ε are real-valued, to re-express the integrals in (78), 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 $\mathrm{dIm}\,\mu_{jk}(\lambda):=(\mathrm{d}\mu_{jk}(\lambda)-\mathrm{d}\mu_{kj}(\lambda))/(2\imath)$. Since $\mathbf{Q}_n$ is a Hermitian projection matrix, we have $[\mathbf{Q}_n\vec{g}_k\cdot\vec{g}_j]=[\overline{\mathbf{Q}}_n\vec{g}_j\cdot\vec{g}_k]$. This implies that the dependence of the measures $\mathrm{dRe}\,\mu_{jk}(\lambda)$ and $\mathrm{dIm}\,\mu_{jk}(\lambda)$ on λ_n and $\mathbf{Q}_n$ are given by

$$\text{(84)}\quad \begin{aligned}\mathrm{dRe}\,\mu_{jk}(\lambda)&=\langle\mathrm{Re}[\mathbf{Q}(\lambda)\vec{g}_j\cdot\vec{g}_k\,]\,\delta_{\lambda_n}(\mathrm{d}\lambda)\rangle, &\mathrm{Re}[\mathbf{Q}(\lambda)\vec{g}_j\cdot\vec{g}_k\,]&=\frac{1}{2}\sum_{n:\,\lambda_n\le\lambda}[(\mathbf{Q}_n+\overline{\mathbf{Q}}_n)\vec{g}_j\cdot\vec{g}_k\,],\\ \mathrm{dIm}\,\mu_{jk}(\lambda)&=\langle\mathrm{Im}[\mathbf{Q}(\lambda)\vec{g}_j\cdot\vec{g}_k\,]\,\delta_{\lambda_n}(\mathrm{d}\lambda)\rangle, &\mathrm{Im}[\mathbf{Q}(\lambda)\vec{g}_j\cdot\vec{g}_k\,]&=\frac{1}{2\imath}\sum_{n:\,\lambda_n\le\lambda}[(\mathbf{Q}_n-\overline{\mathbf{Q}}_n)\vec{g}_j\cdot\vec{g}_k\,].\end{aligned}$$

Moreover, since the eigenvalues $\upsilon_n=\imath\lambda_n$ and eigenvectors $\vec{w}_n$ of the matrix $\mathbf{A}$ come in complex conjugate pairs, the representations of the measures displayed in (84) can be simplified and shown [29] to depend only on the restricted index set $\{n\ge0:\lambda_n\le\lambda\}$. This is clear from equations (78) and (84) since for $n\ge0$ we have $\lambda^2_{-n}=(-\lambda_n)^2=\lambda_n^2$ and from $\vec{w}_{-n}=\overline{\vec{w}_n}$ we also have that $\mathbf{Q}_{-n}=\overline{\mathbf{Q}}_n$. Together, this implies that $\mathrm{Re}[\mathbf{Q}_n\vec{g}_j\cdot\vec{g}_k]+\mathrm{Re}[\mathbf{Q}_{-n}\vec{g}_j\cdot\vec{g}_k]=2\mathrm{Re}[\mathbf{Q}_n\vec{g}_j\cdot\vec{g}_k]$ and $\lambda_n\mathrm{Im}[\mathbf{Q}_n\vec{g}_j\cdot\vec{g}_k]+\lambda_{-n}\mathrm{Im}[\mathbf{Q}_{-n}\vec{g}_j\cdot\vec{g}_k]=2\lambda_n\mathrm{Im}[\mathbf{Q}_n\vec{g}_j\cdot\vec{g}_k]$ with $\lambda_0\mathrm{Im}[\mathbf{Q}_0\vec{g}_j\cdot\vec{g}_k]\equiv0$.

We now show that the integral representations in (78) can be further simplified, due to the projective nature of $\mathbf{\Gamma}$ which causes $\mathbf{A}=\mathbf{\Gamma S\Gamma}$ to have a large null space associated with $\mathbf{\Gamma}$. Moreover, we will also show that the spectral weights associated with this null space are identically zero $[\mathbf{Q}_n\vec{g}_j\cdot\vec{g}_k]\equiv0$. This analysis demonstrates that the computation of these components $\langle\delta_{\lambda_n}(\mathrm{d}\lambda)[\mathbf{Q}_n\vec{g}_j\cdot\vec{g}_k]\rangle$ of the spectral measure $\mathrm{d}\mu_{jk}$ is numerically unstable for $0<\lambda_n\ll1$, if computed directly from the matrix $\mathbf{A}$ using itterative schemes. However, our analysis illustrates a projection method which allows one to compute these components in a relatively stable way. Although, in order to do so, one must perform a complete diagonalization of $\mathbf{\Gamma}$, a *full* matrix, and then a subsequent diagonalization of a smaller matrix, which makes the stable computation of these measure components numerically expensive. For this reason, in Section 7 we will employ the formulation of the effective parameter problem for $\boldsymbol{\mathcal{K}}^*$ given in Corollary 4.1, which involves a *sparse* matrix, which is substantially smaller than that discussed above, in order to compute the integral representations of the components $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ of $\boldsymbol{\mathcal{K}}^*$, and the asymptotics thereof as $\varepsilon\to0$.

In this matrix setting, $\mathbf{\Gamma}$ is a real-symmetric projection matrix of size N satisfying $\mathbf{\Gamma}^T=\mathbf{\Gamma}$ and $\mathbf{\Gamma}^2=\mathbf{\Gamma}$, and its eigenvalues γ_n, $n=1,\ldots,N$, satisfy $\gamma_n=0,1$ [16, 17]. Therefore, $\mathbf{\Gamma}$ has the spectral decomposition $\mathbf{\Gamma}=\mathbf{VGV}^T$, where $\mathbf{V}$ is an orthogonal matrix $\mathbf{VV}^T=\mathbf{V}^T\mathbf{V}=\mathbf{I}$ with columns comprising the eigenvectors of $\mathbf{\Gamma}$, $\mathbf{G}=\mathrm{diag}(\vec{0}_{n_0},\vec{1}_{n_1})$ is a diagonal matrix with the γ_n along its principle diagonal, $\vec{0}_{n_0}$ is a vector of zeros of length n_0, and $\vec{1}_{n_1}$ is a vector of ones of length n_1, with $n_0+n_1=N$. Using this decomposition of $\mathbf{\Gamma}$, we may represent the matrix $\mathbf{A}=\mathbf{\Gamma S\Gamma}$ as $\mathbf{A}=\mathbf{V}(\mathbf{GKG})\mathbf{V}^T$, where $\mathbf{K}=\mathbf{V}^T\mathbf{SV}$ is an anti-symmetric matrix, $\mathbf{K}^T=-\mathbf{K}$, due to the anti-symmetry of the matrix $\mathbf{S}$, $\mathbf{S}^T=-\mathbf{S}$. In block matrix form, we may write the matrices $\mathbf{K}$, $\mathbf{G}$, and $\mathbf{GKG}$ as

$$\text{(85)}\qquad \mathbf{K}=\begin{bmatrix}\mathbf{K}_{00}&\mathbf{K}_{01}\\\mathbf{K}_{10}&\mathbf{K}_{11}\end{bmatrix},\qquad \mathbf{G}=\begin{bmatrix}\mathbf{0}_{00}&\mathbf{0}_{01}\\\mathbf{0}_{10}&\mathbf{I}_{11}\end{bmatrix},\qquad \mathbf{GKG}=\begin{bmatrix}\mathbf{0}_{00}&\mathbf{0}_{01}\\\mathbf{0}_{10}&\mathbf{K}_{11}\end{bmatrix},$$

where $\mathbf{K}_{ab}$ is of size $n_a\times n_b$, $a,b=0,1$, $\mathbf{0}_{ab}$ is a matrix of zeros of size $n_a\times n_b$, and $\mathbf{I}_{aa}$ is the identity matrix of size $n_a\times n_a$. The block matrix form of $\mathbf{GKG}$ in (85) follows directly from that of $\mathbf{K}$ and $\mathbf{G}$, and the properties of block matrix multiplication [8].

Due to the anti-symmetry of $\mathbf{K}$, the matrix $\mathbf{K}_{11}$ is also anti-symmetric and consequently has the spectral decomposition $\mathbf{K}_{11} = \imath\mathbf{U}_{11}\mathbf{\Lambda}_{11}\mathbf{U}_{11}^\dagger$, where $\mathbf{U}_{11}$ is a unitary matrix $\mathbf{U}_{11}^\dagger\mathbf{U}_{11} = \mathbf{U}_{11}\mathbf{U}_{11}^\dagger = \mathbf{I}_{11}$, $\mathbf{\Lambda}_{11}$ is a real-valued diagonal matrix, and the matrix $-\imath\mathbf{K}_{11}$ is Hermitian. We may now write $-\imath\mathbf{GKG}$ in (85) as

$$(86)\qquad -\imath\mathbf{GKG} = \begin{bmatrix} \mathbf{0}_{00} & \mathbf{0}_{01} \\ \mathbf{0}_{10} & \mathbf{U}_{11}\mathbf{\Lambda}_{11}\mathbf{U}_{11}^\dagger \end{bmatrix} = \begin{bmatrix} \mathbf{I}_{00} & \mathbf{0}_{01} \\ \mathbf{0}_{10} & \mathbf{U}_{11} \end{bmatrix} \begin{bmatrix} \mathbf{0}_{00} & \mathbf{0}_{01} \\ \mathbf{0}_{10} & \mathbf{\Lambda}_{11} \end{bmatrix} \begin{bmatrix} \mathbf{I}_{00} & \mathbf{0}_{01} \\ \mathbf{0}_{10} & \mathbf{U}_{11}^\dagger \end{bmatrix} = \mathbf{U\Lambda U}^\dagger,$$

where we have defined $\mathbf{U} = \mathrm{diag}(\mathbf{I}_{00}, \mathbf{U}_{11})$ and $\mathbf{\Lambda} = \mathrm{diag}(\mathbf{0}_{00}, \mathbf{\Lambda}_{11})$. It is easy to see that $\mathbf{U}$ is a unitary matrix, as $\mathbf{U}_{11}$ is unitary. In summary, we have shown that the anti-symmetric matrix $\mathbf{A}$ has the following spectral decomposition

$$(87)\qquad \mathbf{A} = \mathbf{\Gamma S \Gamma} = \imath\mathbf{W\Lambda W}^\dagger, \qquad \mathbf{W} = \mathbf{VU},$$

and since $\mathbf{V}$ is orthogonal and $\mathbf{U}$ is unitary, $\mathbf{W}$ is a unitary matrix $\mathbf{W}^\dagger\mathbf{W} = \mathbf{W}\mathbf{W}^\dagger = \mathbf{I}$.

Equations (86) and (87) show that the eigenvalues $\imath\lambda_n$ of $\mathbf{A}$ are zero $\imath\lambda_n = 0$ for all $n = 1, \dots, n_0$. We now show that the associated spectral weights are also zero $[\mathbf{Q}_n\vec{g}_j \cdot \vec{g}_k] = 0$ for all $n = 1, \dots, n_0$, where $\vec{g}_j = -\mathbf{\Gamma H}\vec{e}_j$, $\mathbf{H}$ is an anti-symmetric matrix, $\mathbf{Q}_n = \vec{w}_n\vec{w}_n^\dagger$, $n = 1, \dots, N$, and $\vec{w}_n$ are the eigenvectors of $\mathbf{A}$ which comprise the columns of the matrix $\mathbf{W}$. From equation (87) we see that $\mathbf{W}^\dagger = \mathbf{U}^\dagger\mathbf{V}^T$. Since $\mathbf{\Gamma} = \mathbf{VGV}^T$ and $\mathbf{V}$ is an orthogonal matrix, this implies that we have $\mathbf{W}^\dagger\mathbf{\Gamma} = \mathbf{U}^\dagger\mathbf{G}\mathbf{V}^T$. Therefore, from the block form of the matrices $\mathbf{G}$ and $\mathbf{U}^\dagger$ displayed in equations (85) and (86), respectively, we see that the block matrix form of $\mathbf{W}^\dagger\mathbf{\Gamma}$ is given by

$$(88)\qquad \mathbf{W}^\dagger\mathbf{\Gamma} = \begin{bmatrix} \mathbf{I}_{00} & \mathbf{0}_{01} \\ \mathbf{0}_{10} & \mathbf{U}_{11}^\dagger \end{bmatrix} \begin{bmatrix} \mathbf{0}_{00} & \mathbf{0}_{01} \\ \mathbf{0}_{10} & \mathbf{I}_{11} \end{bmatrix} \begin{bmatrix} \mathbf{V}_{00}^T & \mathbf{V}_{01}^T \\ \mathbf{V}_{10}^T & \mathbf{V}_{11}^T \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{00} & \mathbf{0}_{01} \\ \mathbf{U}_{11}^\dagger\mathbf{V}_{10}^T & \mathbf{U}_{11}^\dagger\mathbf{V}_{11}^T \end{bmatrix}.$$

Consequently, since $\vec{g}_j = -\mathbf{\Gamma H}\vec{e}_j$, equation (88) implies that $\vec{w}_n^\dagger\vec{g}_j = 0$ for all $n = 1, \dots, n_0$. This, in turn, implies that $[\mathbf{Q}_n\vec{g}_j \cdot \vec{g}_k] = 0$ for all $n = 1, \dots, n_0$, as claimed. This demonstrates that the spectral measure $\mathrm{d}\mu_{jk}(\lambda)$ in (83), underlying the integral representations in (78), do not depend on the components $\langle\delta_{\lambda_n}(\mathrm{d}\lambda)[\mathbf{Q}_n\vec{g}_j \cdot \vec{g}_k]\rangle$ for $n = 1, \dots, n_0$.

4.6. **Finite dimensional matrix setting - Sobelov.** We now formulate the matrix setting associated with Corrolary 4.1, which involves a Sobelov-type inner-product $\langle f, h\rangle_1 = \langle\vec{\nabla} f \cdot \vec{\nabla} h\rangle$. It is more convenient here to consider the weak formulation of the eigenvalue problem $M\varphi_n = \lambda_n\varphi_n$ involving the self-adjoint operator $M = -\imath A$, where the eigenfunction $\varphi_n \in \mathcal{F} \subset \tilde{\mathscr{A}}_\mathcal{T} \otimes \mathcal{H}_\mathcal{V}^1$. From equation (3) we can write $\vec{u} \cdot \vec{\nabla} = \vec{\nabla} \cdot \mathbf{H}\vec{\nabla}$. The matrix representation $\mathbf{M}$ of the operator $M = -\imath\Delta^{-1}(\vec{u} \cdot \vec{\nabla} - \partial_t)$ now follows from our previous discussion, $\mathbf{M} = -\imath\mathbf{\Delta}^{-1}(\mathbf{\nabla H \nabla}^T - \mathbf{D}_t)$. However, even though the matrices $\mathbf{\Delta}^{-1}$ and $\imath(\mathbf{\nabla H \nabla}^T - \mathbf{D}_t)$ are real-symmetric and Hermitian-symmetric, respectively, there composition is not symmetric.

To retain the symmetry properties of the weak form of the eigenvalue problem $M\varphi_n = \lambda_n\varphi_n$, we consider its strong form, which follows by applying the operator Δ to both sides of this formula, yielding

$$(89)\qquad -\imath(\vec{u} \cdot \vec{\nabla} - \partial_t)\varphi_n = \lambda_n\Delta\varphi_n.$$

This formula is well defined for $\varphi_n \in C^1(\mathcal{T}) \otimes C^2(\mathcal{V})$, where $C^k(\Omega)$ denotes the space of continuously differentiable functions of order k with domain Ω. Using equation (89), our goal is to establish discrete integral representations for the functionals $\kappa_{jk}^* = \varepsilon(\delta_{jk} + \langle\chi_j, \chi_k\rangle_1)$ and $\alpha_{jk}^* = \langle A\chi_j, \chi_k\rangle_1$, which are analogous to that in equation (78).

By our previous discussion, the matrix representation of equation (89) is given by

$$(90)\qquad \mathbf{B}\vec{z}_n = \lambda_n\mathbf{C}\vec{z}_n, \qquad \mathbf{B} = -\imath(\mathbf{\nabla}^T\mathbf{H\nabla} - \mathbf{D}_t), \quad \mathbf{C} = \mathbf{\nabla}^T\mathbf{\nabla}.$$

The first formula in equation (90) is a *generalized eigenvalue problem* [28] associated with the pencil $\mathbf{B} - \lambda\mathbf{C}$, where $\mathbf{B}$ and $\mathbf{C}$ are Hermitian-symmetric and real-symmetric matrices, respectively, of size N, say. The λ_n and $\vec{z}_n$, $n=1,\ldots,N$, are known as generalized eigenvalues and eigenvectors, respectively. The matrix $\mathbf{C}=\boldsymbol{\nabla}^T\boldsymbol{\nabla}$ is clearly positive semi-definite. When $\mathbf{C}$ is not positive definite, it can be made so by the method of deflation [28], and we will henceforth assume that $\mathbf{C}$ is positive definite.

Since the matrices $\mathbf{B}$ and $\mathbf{C}$ are symmetric and $\mathbf{C}$ is positive definite, the generalized eigenvalue problem has properties which are similar to those of the standard symmetric eigenvalue problem [28]. In particular, the generalized eigenvalues λ_n are all real and the generalized eigenvectors $\vec{z}_n$ form a basis for $\mathbb{C}^N$, and are orthonormal in the following sense $\vec{z}_n^{\dagger}\mathbf{C}\vec{z}_m=\delta_{nm}$ [28]. Since $\mathbf{C}=\boldsymbol{\nabla}^T\boldsymbol{\nabla}$, this is equivalent to the Sobelov type orthogonality condition

$$\boldsymbol{\nabla}\vec{z}_n\cdot\boldsymbol{\nabla}\vec{z}_m=\delta_{nm},\quad n,m=1,\ldots,N. \tag{91}$$

Denoting $\mathbf{Z}$ the matrix with collumns consisting of the generalized eigenvectors $\vec{z}_n$, equation (91) is seen to be equivalent to $[\boldsymbol{\nabla}\mathbf{Z}]^{\dagger}[\boldsymbol{\nabla}\mathbf{Z}]=\mathbf{I}$, or $\mathbf{Z}^{\dagger}\mathbf{C}\mathbf{Z}=\mathbf{I}$. Moreover, the matrix $\mathbf{Z}$ simultaneously diagonalizes $\mathbf{B}$ and $\mathbf{C}$, i.e. if $\boldsymbol{\Lambda}$ is the diagonal matrix whose diagonal elements are the generalized eigenvalues λ_n, then [28]

$$\mathbf{Z}^{\dagger}\mathbf{B}\mathbf{Z}=\boldsymbol{\Lambda},\qquad \mathbf{Z}^{\dagger}\mathbf{C}\mathbf{Z}=\mathbf{I}. \tag{92}$$

Consider the strong form of the cell problem in (68), $\Delta(\varepsilon+A)\chi_j=-u_j$, and its matrix representation

$$(\varepsilon\mathbf{C}+\imath\mathbf{B})\vec{\chi}_j=-\vec{u}_j. \tag{93}$$

The matrix $\mathbf{Z}$ is invertable, as $\{\vec{z}_n\}$ forms a basis for $\mathbb{C}^N$. Consequently, by equations (92) and (93), we have $\mathbf{B}=\mathbf{Z}^{-\dagger}\boldsymbol{\Lambda}\mathbf{Z}^{-1}$, $\mathbf{C}=\mathbf{Z}^{-\dagger}\mathbf{Z}^{-1}$, and

$$\vec{\chi}_j=\mathbf{Z}(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{Z}^{\dagger}\vec{u}_j. \tag{94}$$

The matrix form of the functionals $\kappa^*_{jk}=\varepsilon(\delta_{jk}+\langle\chi_j,\chi_k\rangle_1)$ and $\alpha^*_{jk}=\langle A\chi_j,\chi_k\rangle_1$ is given by $\kappa^*_{jk}=\varepsilon(\delta_{jk}+\langle\boldsymbol{\nabla}\vec{\chi}_j\cdot\boldsymbol{\nabla}\vec{\chi}_k\rangle)$ and $\alpha^*_{jk}=\langle\boldsymbol{\nabla}\mathbf{C}^{-1}[\imath\mathbf{B}]\vec{\chi}_j\cdot\boldsymbol{\nabla}\vec{\chi}_k\rangle$. Consequently, analogous to the calculation in equation (77), by equation (94) we have

$$\begin{aligned}\kappa^*_{jk}/\varepsilon-\delta_{jk}&=\langle(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{Z}^{\dagger}\vec{u}_j\cdot(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{Z}^{\dagger}\vec{u}_k\rangle\\ \alpha^*_{jk}&=\langle\imath\boldsymbol{\Lambda}(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{Z}^{\dagger}\vec{u}_j\cdot(\varepsilon\mathbf{I}+\imath\boldsymbol{\Lambda})^{-1}\mathbf{Z}^{\dagger}\vec{u}_k\rangle.\end{aligned} \tag{95}$$

A straightforward calculation demonstrates that the functionals in equation (95) have the discrete integral representations of equation (78), under the mappings $\vec{w}_n\mapsto\vec{z}_n$, $\vec{g}_j\mapsto\vec{u}_j$, and $\lambda_n\mapsto-\lambda_n$, so that the spectral weights of the integrals are given by the following formula, which is analogous to equation (79),

$$\overline{(\vec{z}_n^{\dagger}\vec{u}_j)}(\vec{z}_n^{\dagger}\vec{u}_k)=\vec{u}_j^{\,T}\,\vec{z}_n\vec{z}_n^{\dagger}\,\vec{u}_k=\vec{z}_n\vec{z}_n^{\dagger}\vec{u}_j\cdot\vec{u}_k. \tag{96}$$

We now show that a direct correspondence can be made between the discrete integral representation for κ^*_{jk} and α^*_{jk} in (78), with spectral weights given by (96), and that in (35) with the function $\mu_{jk}(\lambda)=\langle Q(\lambda)g_j,g_k\rangle_1$ and $g_j=(-\Delta)^{-1}u_j$. We do so by establishing the analogues of equations (81) and (83) for the current setting. By equation (91), $\{\vec{z}_n\}$ is a basis for $\mathbb{C}^N$ which is orthonormal with respect to the Sobelov type inner-product $\boldsymbol{\nabla}\vec{\xi}\cdot\boldsymbol{\nabla}\vec{\zeta}=[\boldsymbol{\nabla}\vec{\xi}]^{\dagger}[\boldsymbol{\nabla}\vec{\zeta}]$. Consequently, for all $\vec{\xi}\in\mathbb{C}^N$, we have the following analogue of equation (80),

$$\vec{\xi}=\sum_{n=1}^{N}([\boldsymbol{\nabla}\vec{z}_n]^{\dagger}[\boldsymbol{\nabla}\vec{\xi}])\vec{z}_n=\sum_{n=1}^{N}(\vec{z}_n[\boldsymbol{\nabla}\vec{z}_n]^{\dagger}\boldsymbol{\nabla})\vec{\xi}=\sum_{n=1}^{N}\mathbf{Q}_n\vec{\xi},\qquad \mathbf{Q}_n=\vec{z}_n[\boldsymbol{\nabla}\vec{z}_n]^{\dagger}\boldsymbol{\nabla}. \tag{97}$$

This, in turn, establishes the resolution of the identity formula in (81) with $\mathbf{Q}_n=\vec{z}_n[\boldsymbol{\nabla}\vec{z}_n]^{\dagger}\boldsymbol{\nabla}$, which are mutually orthogonal, $\mathbf{Q}_n\mathbf{Q}_m=\mathbf{Q}_n\delta_{nm}$, Hermitian projection matrices.

We now show that the spectral weights in (96) can be written as $\vec{z}_n\vec{z}_n^{\dagger}\vec{u}_j\cdot\vec{u}_k = \boldsymbol{\nabla}\mathbf{Q}_n\vec{g}_j\cdot\boldsymbol{\nabla}\vec{g}_k$, where $\vec{g}_j = (-\boldsymbol{\nabla}^T\boldsymbol{\nabla})^{-1}\vec{u}_j$. Doing so establishes that equation (83) holds with $\mathbf{Q}_n = \vec{z}_n[\boldsymbol{\nabla}\vec{z}_n]^{\dagger}\boldsymbol{\nabla}$ for the current setting. This establishes a direct correspondence between the discrete integral representation for κ^*_{jk} and α^*_{jk} in (78), with spectral weights given by (96), and that in (35) with the function $\mu_{jk}(\lambda) = \langle Q(\lambda)g_j, g_k\rangle_1 = \langle\vec{\nabla}Q(\lambda)g_j\cdot\vec{\nabla}g_k\rangle_1$. Indeed,

$$\vec{z}_n\vec{z}_n^{\dagger}\vec{u}_j\cdot\vec{u}_k = \vec{z}_n\vec{z}_n^{\dagger}[\boldsymbol{\nabla}^T\boldsymbol{\nabla}]\vec{g}_j\cdot[\boldsymbol{\nabla}^T\boldsymbol{\nabla}]\vec{g}_k = [\boldsymbol{\nabla}\vec{z}_n][\boldsymbol{\nabla}\vec{z}_n]^{\dagger}\boldsymbol{\nabla}\vec{g}_j\cdot\boldsymbol{\nabla}\vec{g}_k = \boldsymbol{\nabla}\mathbf{Q}_n\vec{g}_j\cdot\boldsymbol{\nabla}\vec{g}_k. \tag{98}$$

5. Cell flows and Fourier methods

In this section we discuss how Fourier methods can be employed to calculate the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ for a large class of velocity fields $\vec{u}$. It is more natural to focus on the approach discussed in Section 4.2, as opposed to that of Section 4.1, as the underlying operators are *sparse* (infinite) matrices in Fourier space and the velocity field $\vec{u}$ appears naturally, as opposed to the stream matrix $\mathbf{H}$. Our use of Fourier methods in this section is two-fold. In Section 5.1, 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 $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ displayed in equation (72). In Section 5.2, we will apply Fourier methods directly to the cell problem $[\varepsilon\Delta + (\vec{u}\cdot\vec{\nabla} - \partial_t)]\chi_j = -u_j$ of equation (A-9) to obtain infinite series representations of $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$.

5.1. **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 $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$, displayed in equation (72), for a large class of velocity fields $\vec{u}$. In particuar, we consider velocity fields $\vec{u}$ with components u_j, $j = 1,\dots,d$, which are representable by a *finite* number of Fourier modes. More specifically, we consider $\vec{u}\in\mathcal{U}$, where

(99)
$$\mathcal{U} = \otimes_{j=1}^d\mathcal{U}_j, \qquad \mathcal{U}_j = \Big\{u_j\in\mathcal{H}^1 : u_j = \sum_{(\ell,\vec{k})\in I_M^{d+1}} b^j_{\ell,\vec{k}}\,\mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x}\,)}\Big\}, \quad b^j_{\ell,\vec{k}} = \big\langle u_j(t,\vec{x}\,), \mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x}\,)}\big\rangle_2,$$

where $\mathcal{H}^1$ is defined in equation (60), $\vec{k} = (k_1,\dots,k_d)$, and the summation index set I_M^{d+1} is defined as $I_M^{d+1} = \{\vec{q}\in\mathbb{Z}^{d+1} : -M\le q_i\le M,\ M\in\mathbb{N}\}$. It is well known that $\mathcal{U}$ is dense in $\mathcal{H}^1$ [12].

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 $A = \Delta^{-1}(\vec{u}\cdot\vec{\nabla} - \partial_t)$ defined in equation (45). This equation may be rewritten as

$$(\vec{u}\cdot\vec{\nabla} - \partial_t)\varphi_n = \imath\lambda_n\Delta\varphi_n. \tag{100}$$

Since $\varphi_n\in\mathcal{F}\subset\mathcal{H}^1$ and $\{\mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x}\,)} : \ell\in\mathbb{Z},\ \vec{k}\in\mathbb{Z}^d\}$ is an orthonormal basis in $\mathcal{H}^1$ [12] we may represent φ_n by

$$\varphi_n(t,\vec{x}) = \sum_{(\ell,\vec{k})\in\mathbb{Z}^{d+1}} a^n_{\ell,\vec{k}}\,\mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x}\,)}, \tag{101}$$

Inserting this into equation (100) and denoting $\vec{b}_{\ell',\vec{k}} = \big(b^1_{\ell',\vec{k}'},\dots,b^d_{\ell',\vec{k}'}\big)$ the Fourier coefficients of $\vec{u} = (u_1,\dots,u_d)$ in (99) yields

$$\sum_{(\ell,\vec{k})\in\mathbb{Z}^{d+1}} a^n_{\ell,\vec{k}}\,\mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x}\,)}\left(\sum_{(\ell',\vec{k}')\in I_M^{d+1}}\mathrm{e}^{\imath(\ell' t+\vec{k}'\cdot\vec{x}\,)}\left[\vec{b}_{\ell',\vec{k}'}\cdot\imath\vec{k}\right] - \imath\ell + \imath\lambda_n|\vec{k}|^2\right) = 0. \tag{102}$$

Comining, removing the common factor $\imath$, and renumbering the summation involving $\mathrm{e}^{\imath((\ell+\ell')t+(\vec{k}+\vec{k}')\cdot\vec{x})}$ in (102) yields,

$$\sum_{(\ell,\vec{k})\in\mathbb{Z}^{d+1}} \mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x})}\left(\sum_{(\ell',\vec{k}')\in I_M^{d+1}}\left[\vec{b}_{\ell',\vec{k}'}\cdot(\vec{k}-\vec{k}')\right]a^n_{\ell-\ell',\vec{k}-\vec{k}'}-\ell a^n_{\ell,\vec{k}}+\lambda_n|\vec{k}|^2 a^n_{\ell,\vec{k}}\right)=0. \tag{103}$$

Since the orthogonal set $\{\mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x})}:\ell\in\mathbb{Z},\ \vec{k}\in\mathbb{Z}^d\}$ is complete, we have [34, 19] from (103) that

$$\sum_{(\ell',\vec{k}')\in I_M^{d+1}}\left[\vec{b}_{\ell',\vec{k}'}\cdot(\vec{k}-\vec{k}')\right]a^n_{\ell-\ell',\vec{k}-\vec{k}'}-\ell a^n_{\ell,\vec{k}}=-\lambda_n|\vec{k}|^2 a^n_{\ell,\vec{k}}. \tag{104}$$

Equation (104) defines a matrix equation as follows. Define the bijective linear mapping Θ of I_M^{d+1} to $I_M=\{q\in\mathbb{Z}:1\le q_i\le(2M+1)^d,\ M\in\mathbb{N}\}$, $\Theta:I_M^d\mapsto I_M$,

$$\Theta(\ell,\vec{k})=1+\sum_{j=1}^{d}(M+k_j)(2M+1)^{j-1}+(M+\ell)(2M+1)^d \tag{105}$$

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

$$\left\langle \mathrm{e}^{\imath(\ell t+\vec{k}\cdot\vec{x})},\ \mathrm{e}^{\imath(\ell' t+\vec{k}'\cdot\vec{x})}\right\rangle_2=\delta_{\ell,\ell'}\prod_{j=1}^{d}\delta_{k_j,k_j'} \tag{106}$$

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 $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ displayed in equation (72). This representation follows from equations (76), (101), and (106)

$$\langle\varphi_n,g_j\rangle_1=\langle\varphi_n,u_j\rangle_2=\sum_{(\ell',\vec{k}')\in I_M^{d+1}}\overline{a^n_{\ell',\vec{k}'}}\,b^j_{\ell',\vec{k}'} \tag{107}$$

We now discuss how the orthogonality condition $\langle\varphi_n,\varphi_i\rangle_1=\delta_{li}$ in (112) is transformed by the Fourier expansion of the eigenfunctions $\varphi_n(t,\vec{x})$. This expansion of $\varphi_n(t,\vec{x})$ implies that for $\vec{\nabla}\varphi_n(t,\vec{x})$ as follows

$$\varphi_n(t,\vec{x})=\sum_{\ell,m,n}a^l_{\ell,m,n}\mathrm{e}^{\imath(\ell t+mx+ny)}\Rightarrow\vec{\nabla}\varphi_n(t,\vec{x})=\sum_{\ell,m,n}a^l_{\ell,m,n}\,(m,n)\,\mathrm{e}^{\imath(\ell t+mx+ny)}. \tag{108}$$

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 (112) is transformed to

$$\delta_{li}=\langle\vec{\nabla}\varphi_n\cdot\vec{\nabla}\varphi_i\rangle=\sum_{\ell,m,n}(m^2+n^2)\,\overline{a^l_{\ell,m,n}}\,a^i_{\ell,m,n} \tag{109}$$

Recall that $\sum_i i^{-p}$ converges for all $p>1$. From this and equation (109) 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 $m,n\to\pm\infty$. Since $\varphi_n(\cdot,\vec{x})\in\tilde{\mathscr{A}}_{\mathcal{T}}(\mathcal{T})$, i.e. $\partial_t\varphi_n(\cdot,\vec{x})\in L^2(\mathcal{T})$, we also have $|a^l_{\ell,m,n}|^2\sim o(\ell^{-3})$ as $\ell\to\pm\infty$. Since $\partial_t\vec{\nabla}\varphi_n\in L^2(\mathcal{T}\times\mathcal{V})$ we may generalize both of these statements by the following

$$|a^l_{\ell,m,n}|^2\sim o(\ell^{-3}(m^2+n^2)^{-3/2}),\ \text{as}\ \ \ell,m,n\to\pm\infty. \tag{110}$$

5.2. **Direct methods.**

5.3. **Special cases.** 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 $A = (-\Delta)^{-1}(\partial_t + \vec{u}\cdot\vec{\nabla})$, introduced in equation (45) of our (attached) effective-diffusivity paper, with $\vec{u} \mapsto -\vec{u}$. Here A is an anti-symmetric (normal) operator and the incompressible velocity field $\vec{u}(t, \vec{x})$ is given in equation (124) above. The equation $A\varphi_n = \imath\lambda_n\varphi_n$ may be rewritten as

$$(\partial_t + \vec{u}\cdot\vec{\nabla})\varphi_n = -\imath\lambda_n\Delta\varphi_n. \tag{111}$$

The eigenfunctions φ_n satisfy the following orthogonality condition

$$\langle\varphi_n, \varphi_i\rangle_1 = \langle\vec{\nabla}\varphi_n \cdot \vec{\nabla}\varphi_i\rangle = \delta_{li}, \tag{112}$$

where δ_{li} is the Kronecker delta and $\langle\cdot\rangle$ denotes space-time averaging over the period cell $\mathcal{T} \times \mathcal{V}$, with $\mathcal{T} = [0, 2\pi]$ and $\mathcal{V} = [0, 2\pi] \times [0, 2\pi]$.

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

$$\mathcal{F} = \{f \in \tilde{\mathscr{A}}_{\mathcal{T}}(\mathcal{T}) \otimes \mathcal{H}^1(\mathcal{V}) \,|\, \langle f\rangle = 0 \text{ and is periodic on } \mathcal{T}\times\mathcal{V}\}. \tag{113}$$

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

$$\varphi_n(t, \vec{x}) = \sum_\ell \varphi^l_\ell(\vec{x})\, e^{\imath\ell t}, \tag{114}$$

where $\varphi^l_\ell \in \mathcal{H}^1(\mathcal{V})$. Write $\cos t = (e^{\imath t} + e^{-\imath t})/2$ and insert this and (114) into equation (111), yielding

$$\sum_\ell(\imath\ell + \vec{u}_1\cdot\vec{\nabla} + \imath\lambda_n\Delta)\varphi^l_\ell(\vec{x})e^{\imath\ell t} + \frac{\delta}{2}\sum_\ell(e^{\imath(\ell+1)t} + e^{\imath(\ell-1)t})\,\vec{u}_2\cdot\vec{\nabla}\varphi^l_\ell(\vec{x}) = 0, \tag{115}$$

or:

$$\sum_\ell\left[(\imath\ell + \vec{u}_1\cdot\vec{\nabla} + \imath\lambda_n\Delta)\varphi^l_\ell(\vec{x}) + \frac{\delta}{2}\vec{u}_2\cdot\vec{\nabla}(\varphi^l_{\ell-1}(\vec{x}) + \varphi^l_{\ell+1}(\vec{x}))\right]e^{\imath\ell t} = 0. \tag{116}$$

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

$$(\imath\ell + \vec{u}_1\cdot\vec{\nabla})\varphi^l_\ell(\vec{x}) + \frac{\delta}{2}\vec{u}_2\cdot\vec{\nabla}(\varphi^l_{\ell-1}(\vec{x}) + \varphi^l_{\ell+1}(\vec{x})) = -\imath\lambda_n\Delta\varphi^l_\ell(\vec{x}). \tag{117}$$

The system of partial differential equations in (117) can be reduced to a system of algebraic equations as follows. Recall that $\vec{u}_1(\vec{x}) = (\cos y, \cos x)$ and $\vec{u}_2(\vec{x}) = (\sin y, \sin x)$, which implies

$$\begin{aligned}(\vec{u}_1\cdot\vec{\nabla})\varphi^l_\ell(\vec{x}) &= \cos y\,\partial_x\varphi^l_\ell(\vec{x}) + \cos x\,\partial_y\varphi^l_\ell(\vec{x})\\ (\vec{u}_2\cdot\vec{\nabla})\varphi^l_\ell(\vec{x}) &= \sin y\,\partial_x\varphi^l_\ell(\vec{x}) + \sin x\,\partial_y\varphi^l_\ell(\vec{x})\end{aligned} \tag{118}$$

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

$$\varphi^l_\ell(\vec{x}) = \sum_{m,n} a^l_{\ell,m,n}\, e^{\imath(mx+ny)} \tag{119}$$

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 (142) into equation (118), yielding

$$\begin{aligned}(120)\qquad &(\vec{u}_1\cdot\vec{\nabla})\varphi_\ell^l\\ &\quad=\frac{1}{2}\sum_{m,n}a_{\ell,m,n}^l\left[\imath m\,\mathrm{e}^{\imath mx}(\mathrm{e}^{\imath(n+1)y}+\mathrm{e}^{\imath(n-1)y})+\imath n\,\mathrm{e}^{\imath ny}(\mathrm{e}^{\imath(m+1)x}+\mathrm{e}^{\imath(m-1)x})\right]\\ &(\vec{u}_2\cdot\vec{\nabla})\varphi_\ell^l\\ &\quad=\frac{1}{2\imath}\sum_{m,n}a_{\ell,m,n}^l\left[\imath m\,\mathrm{e}^{\imath mx}(\mathrm{e}^{\imath(n+1)y}-\mathrm{e}^{\imath(n-1)y})+\imath n\,\mathrm{e}^{\imath ny}(\mathrm{e}^{\imath(m+1)x}-\mathrm{e}^{\imath(m-1)x})\right]\end{aligned}$$

or:

$$(\vec{u}_1\cdot\vec{\nabla})\varphi_\ell^l=\frac{\imath}{2}\sum_{m,n}[m(a_{\ell,m,n-1}^l+a_{\ell,m,n+1}^l)+n(a_{\ell,m-1,n}^l+a_{\ell,m+1,n}^l)]\mathrm{e}^{\imath(mx+ny)}$$

$$(\vec{u}_2\cdot\vec{\nabla})\varphi_\ell^l=\frac{1}{2}\sum_{m,n}[m(a_{\ell,m,n-1}^l-a_{\ell,m,n+1}^l)+n(a_{\ell,m-1,n}^l-a_{\ell,m+1,n}^l)]\mathrm{e}^{\imath(mx+ny)}. \tag{121}$$

We also have

$$-\Delta\varphi_\ell^l=\sum_{m,n}a_{\ell,m,n}^l(m^2+n^2)\mathrm{e}^{\imath(mx+ny)} \tag{122}$$

By the completeness of the orthogonal set $\{\mathrm{e}^{\imath(mx+ny)}\}$, inserting equations (121) and (122) into equation (117) yields

$$\begin{aligned}&\imath\ell\,a_{\ell,m,n}^l+\frac{\imath}{2}[m(a_{\ell,m,n-1}^l+a_{\ell,m,n+1}^l)+n(a_{\ell,m-1,n}^l+a_{\ell,m+1,n}^l)]\\ &\qquad+\frac{\delta}{4}[m(a_{\ell-1,m,n-1}^l-a_{\ell-1,m,n+1}^l)+n(a_{\ell-1,m-1,n}^l-a_{\ell-1,m+1,n}^l)\\ &\qquad\quad+m(a_{\ell+1,m,n-1}^l-a_{\ell+1,m,n+1}^l)+n(a_{\ell+1,m-1,n}^l-a_{\ell+1,m+1,n}^l)]\\ &\quad=\imath\lambda_n(m^2+n^2)a_{\ell,m,n}^l,\end{aligned} \tag{123}$$

which is an infinite system of algebraic equations for the unknown Fourier coefficients $a_{\ell,m,n}^l$ associated with the eigenfunctions $\varphi_n(t,\vec{x})$ 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 (124) and the Fourier expansion of the eigenfunctions φ_n in (108) allow the spectral weights $\langle\varphi_n,g_j\rangle$ in equation (72) to be given in terms of the Fourier coefficients $a_{\ell,m,n}^l$ for the reduced index set $\ell,m,n\in\{-1,0,1\}$.

$$\vec{u}(t,\vec{x})=(\cos y,\cos x)+\delta\cos t\,(\sin y,\sin x):=\vec{u}_1(\vec{x})+\delta\cos t\;\vec{u}_2(\vec{x}). \tag{124}$$

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 (124) we have that

$$\begin{aligned}u_1(t,x,y)&=\cos y+\cos t\sin y\\ &=\frac{1}{2}\left(\mathrm{e}^{\imath y}+\mathrm{e}^{-\imath y}\right)+\frac{1}{4\imath}\left(\mathrm{e}^{\imath t}+\mathrm{e}^{-\imath t}\right)(\mathrm{e}^{\imath y}-\mathrm{e}^{-\imath y})\\ &=\frac{1}{2}\left(\mathrm{e}^{\imath y}+\mathrm{e}^{-\imath y}\right)+\frac{1}{4\imath}\left(\mathrm{e}^{\imath(t+y)}-\mathrm{e}^{\imath(t-y)}+\mathrm{e}^{\imath(-t+y)}-\mathrm{e}^{\imath(-t-y)}\right),\end{aligned} \tag{125}$$

and $u_2(t,x,y) = u_1(t,y,x)$. This, equation (76), and the orthogonality relation in (106) imply that

$$\begin{aligned} \langle\varphi_n, g_1\rangle_1 &= \frac{1}{2}\left(a^{\,l}_{0,0,1} + a^{\,l}_{0,0,-1}\right) + \frac{1}{4\imath}\left(a^{\,l}_{1,0,1} - a^{\,l}_{1,0,-1} + a^{\,l}_{-1,0,1} - a^{\,l}_{-1,0,-1}\right) \\ \langle\varphi_n, g_2\rangle_1 &= \frac{1}{2}\left(a^{\,l}_{0,1,0} + a^{\,l}_{0,-1,0}\right) + \frac{1}{4\imath}\left(a^{\,l}_{1,1,0} - a^{\,l}_{1,-1,0} + a^{\,l}_{-1,1,0} - a^{\,l}_{-1,-1,0}\right) \end{aligned} \tag{126}$$

Since $\vec{u}_i$ is incompressible, there exists an anti-symmetric matrix $\mathbf{H}_i$ such that $\vec{u}_i = \vec{\nabla}\cdot\mathbf{H}_i$. This allows us to write $\vec{u}_i\cdot\vec{\nabla} = \vec{\nabla}\cdot\mathbf{H}_i\vec{\nabla}$, which is an anti-symmetric operator. When $\delta = 0$, the velocity field $\vec{u}$ is time-independent and the operator A, which arises from the cell problem, becomes $A = (-\Delta)^{-1}(\vec{u}_1\cdot\vec{\nabla})$. In this case, the eigenvalue problem in (111) becomes

$$\vec{\nabla}\cdot\mathbf{H}_1\vec{\nabla}\varphi = \lambda\Delta\varphi. \tag{127}$$

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 $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$, displayed in equation (35) of our (attached) paper.

5.4. **Matrix representations of the eigenvalue problem.** In the *time-independent case*, where $\delta = 0$ in the velocity field of equation (124), the system of equations in (123) corresponding to the eigenvalue problem becomes

$$m(a_{m,n-1} + a_{m,n+1}) + n(a_{m-1,n} + a_{m+1,n}) = 2\lambda(m^2+n^2)a_{m,n}, \quad m,n\in\mathbb{Z}, \tag{128}$$

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 (128) 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

$$B\vec{a}_l = 2\lambda_n C\vec{a}_l, \tag{129}$$

where B and C are $(2M+1)^2\times(2M+1)^2$ symmetric matrices and $l = 1,\dots,(2M+1)^2$. More specifically, B is real-symmetric and C is real-diagonal positive-semi-definite. Equation (129) 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 $\vec{a}_l$ – consisting of the Fourier coefficients for φ_n – satisfy the orthogonality condition

$$\vec{a}_j^{\,T} C\vec{a}_k = \delta_{jk}. \tag{130}$$

The rows and columns of B and C, corresponding to the $a_{0,0}$ component of $\vec{a}$, 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 $\delta \ne 0$ in the velocity field of equation (124), slightly manipulating equation (123) yields

$$\begin{aligned} &4\ell\, a_{\ell,m,n} + 2[m(a_{\ell,m,n-1} + a_{\ell,m,n+1}) + n(a_{\ell,m-1,n} + a_{\ell,m+1,n})] \\ &\qquad -\imath\delta[m(a_{\ell-1,m,n-1} - a_{\ell-1,m,n+1} + a_{\ell+1,m,n-1} - a_{\ell+1,m,n+1}) \\ &\qquad\quad + n(a_{\ell-1,m-1,n} - a_{\ell-1,m+1,n} + a_{\ell+1,m-1,n} - a_{\ell+1,m+1,n})] \\ &\quad = 4\lambda(m^2+n^2)a_{\ell,m,n}. \end{aligned} \tag{131}$$

By restricting the indices, $-M \le l,m,n \le M$, in equation (131) and imposing suitable boundary conditions, it can also be written as the generalized eigenvalue problem of equations (129) and (130), where B and C are $(2M+1)^3\times(2M+1)^3$ symmetric matrices. More specifically, B is Hermitian-symmetric and C is real-diagonal. The rows and columns of B and C, corresponding to the $a_{0,0,0}$

component of $\vec{a}$, consist entirely of zero elements. Therefore, without loss of generality, they can be removed from the generalized eigenvalue problem, making the matrix C positive-definite.

5.5. **Three-Dim Steady Cellular Flows.** The 3 dimensional (3D) steady cellular flows are:

$$B = (\Phi_x(x,y)W'(z), \Phi_y(x,y)W'(z), k\Phi(x,y)W(z)), \tag{132}$$

with $-\Delta\Phi = k\Phi$.

A special case is $k = 2$, then

$$\vec{u}(x,y,z) = (-\sin x\, \cos y\, \cos z, -\cos x\, \sin y\, \cos z, 2\cos x\, \cos y\, \sin z). \tag{133}$$

We now derive a system of algebraic equations, analogous to that of equation (123), corresponding to the velocity field $\vec{u}$ displayed in (133). The steady state eigenvalue problem of equation (111) is given by

$$\vec{u}\cdot\vec{\nabla}\varphi_n = -\imath\lambda_n\Delta\varphi_n. \tag{134}$$

The analog of equation (118) is

$$(\vec{u}\cdot\vec{\nabla})\varphi_n(\vec{x}) = -\sin x\, \cos y\, \cos z\, \partial_x\varphi_n(\vec{x}) - \cos x\, \sin y\, \cos z\, \partial_y\varphi_n(\vec{x}) + 2\cos x\, \cos y\, \sin z\, \partial_z\varphi_n(\vec{x}). \tag{135}$$

For this three dimensional flow, we use the following notation for the Fourier expansion of $\varphi_n(\vec{x})$:

$$\varphi_n(\vec{x}) = \sum_{\ell,m,n} a^{l}_{\ell,m,n}\mathrm{e}^{\imath(\ell x+my+nz)}. \tag{136}$$

Using the identities

$$\begin{aligned}
u_1(\vec{x}) &= -\sin x\, \cos y\, \cos z = -\frac{1}{4}(+\sin(x-y-z)+\sin(x-y+z)+\sin(x+y-z)+\sin(x+y+z))\\
u_2(\vec{x}) &= -\cos x\, \sin y\, \cos z = \frac{1}{4}(+\sin(x-y-z)+\sin(x-y+z)-\sin(x+y-z)-\sin(x+y+z))\\
u_3(\vec{x}) &= 2\cos x\, \cos y\, \sin z = \frac{1}{2}(-\sin(x-y-z)+\sin(x-y+z)-\sin(x+y-z)+\sin(x+y+z)),
\end{aligned} \tag{137}$$

and writing $\sin x = (\mathrm{e}^{\imath x} - \mathrm{e}^{-\imath x})/(2\imath)$, for example, one can more easily see that the analogue of equation (123) for the velocity field in (133) is given by

$$\begin{aligned}
&-\frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m+1,n+1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m-1,n-1} - \frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m+1,n-1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m-1,n+1}\\
&-\frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m-1,n+1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m+1,n-1} - \frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m-1,n-1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m+1,n+1}\\
&\frac{\imath(m+1)}{8\imath}a_{\ell-1,m+1,n+1} - \frac{\imath(m-1)}{8\imath}a_{\ell+1,m-1,n-1} + \frac{\imath(m+1)}{8\imath}a_{\ell-1,m+1,n-1} - \frac{\imath(m-1)}{8\imath}a_{\ell+1,m-1,n+1}\\
&-\frac{\imath(m-1)}{8\imath}a_{\ell-1,m-1,n+1} + \frac{\imath(m+1)}{8\imath}a_{\ell+1,m+1,n-1} - \frac{\imath(m-1)}{8\imath}a_{\ell-1,m-1,n-1} + \frac{\imath(m+1)}{8\imath}a_{\ell+1,m+1,n+1}\\
&-\frac{\imath(n+1)}{4\imath}a_{\ell-1,m+1,n+1} + \frac{\imath(n-1)}{4\imath}a_{\ell+1,m-1,n-1} + \frac{\imath(n-1)}{4\imath}a_{\ell-1,m+1,n-1} - \frac{\imath(n+1)}{4\imath}a_{\ell+1,m-1,n+1}\\
&-\frac{\imath(n+1)}{4\imath}a_{\ell-1,m-1,n+1} + \frac{\imath(n-1)}{4\imath}a_{\ell+1,m+1,n-1} + \frac{\imath(n-1)}{4\imath}a_{\ell-1,m-1,n-1} - \frac{\imath(n+1)}{4\imath}a_{\ell+1,m+1,n+1}\\
&=\imath\lambda_n(m^2+n^2)a_{\ell,m,n},
\end{aligned} \tag{138}$$

where we have suppressed the super-script notation and written $a^l_{\ell,m,n} = a_{\ell,m,n}$. Simplifying equation (138) yields

$$
\begin{aligned}
&\imath((\ell-1)-(m+1)+2(n+1))a_{\ell-1,m+1,n+1}+\imath(-(\ell+1)+(m-1)-2(n-1))a_{\ell+1,m-1,n-1}\\
&+\imath((\ell-1)-(m+1)-2(n-1))a_{\ell-1,m+1,n-1}+\imath(-(\ell+1)+(m-1)+2(n+1))a_{\ell+1,m-1,n+1}\\
&+\imath((\ell-1)+(m-1)+2(n+1))a_{\ell-1,m-1,n+1}+\imath(-(\ell+1)-(m+1)-2(n-1))a_{\ell+1,m+1,n-1}\\
&+\imath((\ell-1)+(m-1)-2(n-1))a_{\ell-1,m-1,n-1}+\imath(-(\ell+1)-(m+1)+2(n+1))a_{\ell+1,m+1,n+1}\\
&=8\lambda_n(m^2+n^2)a_{\ell,m,n},
\end{aligned}
\tag{139}
$$

From equations (76) and (137), one can see that the analogue of equation (126) is given by

$$
\begin{aligned}
\langle\varphi_n,g_1\rangle_1 &= -\frac{1}{8\imath}\left(+(a_{1,-1,-1}-a_{-1,1,1})+(a_{1,-1,1}-a_{-1,1,-1})+(a_{1,1,-1}-a_{-1,-1,1})+(a_{1,1,1}-a_{-1,-1,-1})\right)\\
\langle\varphi_n,g_2\rangle_1 &= \frac{1}{8\imath}\left(+(a_{1,-1,-1}-a_{-1,1,1})+(a_{1,-1,1}-a_{-1,1,-1})-(a_{1,1,-1}-a_{-1,-1,1})-(a_{1,1,1}-a_{-1,-1,-1})\right)\\
\langle\varphi_n,g_3\rangle_1 &= \frac{1}{4\imath}\left(-(a_{1,-1,-1}-a_{-1,1,1})+(a_{1,-1,1}-a_{-1,1,-1})-(a_{1,1,-1}-a_{-1,-1,1})+(a_{1,1,1}-a_{-1,-1,-1})\right)
\end{aligned}
\tag{140}
$$

By restricting the indices, $-M \le l, m, n \le M$, in equation (139) and imposing suitable boundary conditions, it can also be written as the generalized eigenvalue problem of equations (129) and (130), where B and C are $(2M+1)^3 \times (2M+1)^3$ symmetric matrices. More specifically, B is Hermitian-symmetric and C is real-diagonal positive-semi-definite. The rows and columns of B and C, corresponding to the $a_{0,0,0}$ component of $\vec{a}$, consist entirely of zero elements. Therefore, without loss of generality, they can be removed from these matrices, making the matrix C positive-definite.

5.5.1. *Another formulation.* We can compute the components of the effective diffusivity tensor directly using only Fourier methods, as opposed to using Fourier methods and spectral methods in concert. Consider the cell problem of equation (68), $(\varepsilon + A)\chi_j = g_j$, which involves the function $\chi_j(t,\vec{x})$ which is a member of the function space $\mathcal{F}$ defined in equation (113), $\chi_j \in \mathcal{F}$, which we take to be 2π space-time periodic. Here, $A = (-\Delta)^{-1}(\partial_t + \vec{u}\cdot\vec{\nabla})$, $g_j = (-\Delta)^{-1}u_j$, and u_j is the jth component, $j = 1, 2$, of the velocity field $\vec{u}$. Consequently, the cell problem is equivalent to

$$(\partial_t + \vec{u}\cdot\vec{\nabla} - \varepsilon\Delta)\chi_j(t,\vec{x}) = u_j(t,\vec{x}) \tag{141}$$

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

$$\chi_j(t,\vec{x}) = \sum_{m,n} b^j_{m,n}(t)\, e^{\imath(mx+ny)}, \quad b^j_{m,n}(0) = b^j_{m,n}(2\pi) \tag{142}$$

Inserting this into equation (**??**) yields

$$\sum_{m,n} e^{\imath(mx+ny)}[\partial_t + \imath m u_1 + \imath n u_2 + \varepsilon(m^2+n^2)]b^j_{m,n} = u_j \tag{143}$$

Consider the velocity field $\vec{u} = (u_1, u_2)$ defined in equation (124), so that $u_1 = \cos y + \delta\cos t\,\sin y$ and $u_2 = \cos y + \delta\cos t\,\sin y$. Write $\cos x = (e^{\imath x} + e^{-\imath x})/2$ and $\sin x = (e^{\imath x} - e^{-\imath x})/(2\imath)$, for example.

In view of equations (120) and (121), equation (143) can be written as

$$\sum_{m,n} \mathrm{e}^{\imath(mx+ny)}[\partial_t b^1_{m,n} + \frac{\imath}{2}(m(b^1_{m,n-1} + b^1_{m,n+1}) + n(b^1_{m-1,n} + b^1_{m+1,n})) + \frac{\delta\cos t}{2}(m(b^1_{m,n-1} - b^1_{m,n+1}) + n(b^1_{m-1,n} - b^1_{m+1,n})) + \varepsilon(m^2+n^2)b^1_{m,n} - \frac{1}{2}\delta_{0,m}(\delta_{1,n} + \delta_{-1,n}) - \frac{\delta\cos t}{2\imath}\delta_{0,m}(\delta_{1,n} - \delta_{-1,n})] = 0. \tag{144}$$

Since $u_2(t,x,y) = u_1(t,y,x)$, the analogous formula involving $b^2_{m,n}$ follows from interchanging $\delta_{l,m}$ with $\delta_{l,n}$ in (144), $l = -1, 0, 1$, where $\delta_{l,m}$ is the Kronecker delta. By the completeness of the orthogonal set $\{\mathrm{e}^{\imath(mx+ny)}\}$ and equation (144), we have that the cell problem in (**??**) is equivalent to the following two (infinite) linear systems of coupled ordinary differential equations (ODE's)

$$\begin{aligned} \partial_t b^1_{m,n} &+ \frac{\imath}{2}(m(b^1_{m,n-1} + b^1_{m,n+1}) + n(b^1_{m-1,n} + b^1_{m+1,n})) \\ &+ \frac{\delta\cos t}{2}(m(b^1_{m,n-1} - b^1_{m,n+1}) + n(b^1_{m-1,n} - b^1_{m+1,n})) + \varepsilon(m^2+n^2)b^1_{m,n} \\ &= \frac{1}{2}\delta_{0,m}(\delta_{1,n} + \delta_{-1,n}) + \frac{\delta\cos t}{2\imath}\delta_{0,m}(\delta_{1,n} - \delta_{-1,n}), \\ \partial_t b^2_{m,n} &+ \frac{\imath}{2}(m(b^2_{m,n-1} + b^2_{m,n+1}) + n(b^2_{m-1,n} + b^2_{m+1,n})) \\ &+ \frac{\delta\cos t}{2}(m(b^2_{m,n-1} - b^2_{m,n+1}) + n(b^2_{m-1,n} - b^2_{m+1,n})) + \varepsilon(m^2+n^2)b^2_{m,n} \\ &= \frac{1}{2}\delta_{0,n}(\delta_{1,m} + \delta_{-1,m}) + \frac{\delta\cos t}{2\imath}\delta_{0,n}(\delta_{1,m} - \delta_{-1,m}), \end{aligned} \tag{145}$$

with initial condition $b^j_{m,n}(0) = b^j_{m,n}(2\pi)$, $j = 1,2$, $m,n \in \mathbb{Z}$. For each $j = 1,2$, when the indices in equation (145) are restricted to be finite, $-M \le m,n \le M$ say, and suitable boundary conditions are imposed, the *infinite* system of ODE's reduce to a *finite* system of ODE's. In this case, each of the two systems can be simulated for $t \in [0, 2\pi]$ to obtain the trajectories of the $b^j_{m,n}(t)$, $j = 1,2$, $-M \le m,n \le M$. The behavior of these Fourier coefficients, in turn, lead to computations of the components of the effective diffusivity tensor.

Before we describe how the components of the effective diffusivity tensor are computed from the behavior of the Fourier coefficients $b^j_{m,n}(t)$, we discuss the case where $\delta = 0$, so that the velocity field in (124) is time-independent. In this case, equation (145) reduces to the following linear, algebraic system

$$\begin{aligned} \frac{\imath}{2}(m(b^1_{m,n-1} + b^1_{m,n+1}) + n(b^1_{m-1,n} + b^1_{m+1,n})) + \varepsilon(m^2+n^2)b^1_{m,n} &= \frac{1}{2}\delta_{0,m}(\delta_{1,n} + \delta_{-1,n}) \\ \frac{\imath}{2}(m(b^2_{m,n-1} + b^2_{m,n+1}) + n(b^2_{m-1,n} + b^2_{m+1,n})) + \varepsilon(m^2+n^2)b^2_{m,n} &= \frac{1}{2}\delta_{0,n}(\delta_{1,m} + \delta_{-1,m}). \end{aligned} \tag{146}$$

When the indices of equation (146) 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

$$(B + \varepsilon C)\vec{b}^j = \vec{\xi}^j \tag{147}$$

The rows and columns of B and C, corresponding to the $b^j_{0,0}$ component of the unknown vector $\vec{b}^j$, consist entirely of zero elements. Therefore, without loss of generality, they can be removed from these matrices, making the matrix C positive-definite. Consequently, for each $\varepsilon > 0$, this algebraic system can be directly and *simultaneously* solved for $j = 1,2$ using techniques of linear algebra, to determine the Fourier coefficients of χ_j in $\vec{b}^j$.

We now discuss how the behavior of the Fourier coefficients $b^j_{m,n}$ of χ_j lead to computations of the effective diffusivity tensor. Recall that the components $\kappa^*_{jk} = \varepsilon(\delta_{jk}+\langle\chi_j,\chi_k\rangle_1)$ and $\alpha^*_{jk} = \langle A\chi_j,\chi_k\rangle_1$ of the effective tensors $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ are given in equation (**??**). Here, $\langle\chi_j,\chi_k\rangle_1 = \langle\vec{\nabla}\chi_j\cdot\vec{\nabla}\chi_k\rangle$, for example, and $\langle\cdot\rangle$ denotes space-time averaging. From equations (106), (109), and (142) we have

$$\langle\chi_j,\chi_k\rangle_1 = \sum_{m,n}(m^2+n^2)\,\langle\overline{b^j_{m,n}}\,b^k_{m,n}\rangle_t, \tag{148}$$

where $\langle\cdot\rangle_t$ denotes time averaging. In the case of a time-independent velocity field, when $\delta = 0$, the Fourier coefficients $b^j_{m,n}$ are also time-independent, so that $\langle\overline{b^j_{m,n}}\,b^k_{m,n}\rangle_t = \overline{b^j_{m,n}}\,b^k_{m,n}$. From equation (76) we have that $\langle A\chi_j,\chi_k\rangle_1 = \langle(\partial_t+\vec{\nabla}\cdot\vec{u})\chi_j,\chi_k\rangle_2$, where $\langle\cdot,\cdot\rangle_2$ denotes the $L^2(\mathcal{T},\mathcal{V})$ inner-product. Consequently, from equation (144) we have

(149)

$$\langle A\chi_j,\chi_k\rangle_1 = \sum_{m,n}\langle\overline{\gamma^{\delta,j}_{m,n}}\,b^k_{m,n}\rangle_t, \quad \gamma^{\delta,j}_{m,n} = \partial_t b^j_{m,n} + \frac{\imath}{2}(m(b^j_{m,n-1}+b^j_{m,n+1}) + n(b^j_{m-1,n}+b^j_{m+1,n})) + \frac{\delta\cos t}{2}(m(b^j_{m,n-1}-b^j_{m,n+1}) + n(b^j_{m-1,n}-b^j_{m+1,n})).$$

In the case of a time-independent velocity field, when $\delta = 0$, the Fourier coefficients $b^j_{m,n}$ are also time-independent, so that $\langle\overline{\gamma^{\delta,j}_{m,n}}\,b^k_{m,n}\rangle_t = \overline{\gamma^{\delta,j}_{m,n}}\,b^k_{m,n}$ and $\gamma^{\delta,j}_{m,n} = (m(b^j_{m,n-1}+b^j_{m,n+1}) + n(b^j_{m-1,n} + b^j_{m+1,n}))/(-2\imath)$.

6. Spectral and asymptotic analysis of effective diffusivity

In Section 4 we derived the Radon–Stieltjes integral representations for the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ displayed in equation (35), involving a spectral measure $\mathrm{d}\boldsymbol{\mu}$ associated with the operator $\mathbf{A}$ on the function space $\mathscr{F}$ described in Theorem 2.1, or equivalently the operator A on the function space $\mathcal{F}$ described in Corollary 4.1, as discussed in Theorem 4.2. There, we briefly discussed that the domain of integration of these representations are determined by the spectrum $\Sigma(\mathbf{A})$ of the operator $\mathbf{A}$, for example. In this section we discuss the properties of $\Sigma(\mathbf{A})$ in more detail and use this important information to provide various decompositions of the measure $\mathrm{d}\boldsymbol{\mu}$ which provides asymptotic behavior of the components κ^*_{jk} and α^*_{jk}, $j,k = 1,\dots,d$, as the molecular diffusivity $\varepsilon\to 0$.

7. Numerical Results

In this section we discuss the numerical implementation of the integral representations in equation (78), involving the signed, discrete measures displayed in (84). In particular, we directly compute the spectral measure $\mathrm{d}\boldsymbol{\mu}(\lambda)$ associated with discretizations of velocity fields $\vec{u}$ for model flows, to compute the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the associated effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$. We explore the numerical implementation of the different formulations of the effective parameter problem, described by Corollary 4.1 and Theorem 4.1 which involve the anti-symmetric operators A and $\mathbf{A}$, respectively. This analysis demonstrates that formulation described by Corollary 4.1 provides a more practical numerical implementation than that described in Theorem 4.1, as A is a *sparse* matrix of size N, say, and $\mathbf{A}$ is a *full* matrix of size dN.

A-1. Appendix

A-1.1. **The flow matrix H.** THIS SECTION IS UNDER CONSTRUCTION

A-1.2. **Multiple scale method.** In this section we provide the details of the multiple scale method [21, 26, 27, 4] which leads to equations (6)–(9). We assume that equation (1) has already been non-dimensionalized so that $\kappa_0 \mapsto \varepsilon$ and $\vec{v} \mapsto \vec{u}$. The key assumption of the method is that the initial density ϕ_0 in (1) is slowly varying relative to the velocity field $\vec{u}$, which introduces a small parameter $\delta \ll 1$ such that

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

The variable changes $\vec{x} \mapsto \vec{y} = \vec{x}/\delta$ and $t \mapsto \tau = t/\delta^2$, along with equations (2) and (A-2), transforms equation (1) into [21]

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

We now expand ϕ^δ in powers of δ [21]

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

Writing

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

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

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

Inserting this into equation (A-3) and setting the coefficients associated with the various powers of δ to zero, yields a sequence of problems.

Due to the dependence of $\bar{\phi}(t, \vec{x})$ 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

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

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

By the linearity of equation (A-6), we may separate the fast and slow variables by writing [21]

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

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

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

equation (A-6) is automatically satisfied [21]. Equation (A-9) along with (3) is equivalent to the cell problem (7), where the distinction of fast variables was dropped for notational simplicity. In order for $\phi^{(1)}(t, \vec{x}, \tau, \vec{y})$ in (A-8) to be periodic in $(\tau, \vec{y})$ for each fixed $(t, \vec{x})$, we must have that the functions $\chi_k(\tau, \vec{y})$, $k = 1, \ldots, d$, are periodic. This and the fundamental theorem of calculus implies that $\langle\vec{\nabla}_y\chi_k\rangle = 0$. Here, $\langle\cdot\rangle$ denotes space-time averaging with respect to the *fast variables*.

Due to the incompressibility of the velocity field $\vec{\nabla}_y \cdot \vec{u}(\tau, \vec{y}) = 0$ 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 $\langle\vec{u}\rangle = 0$ and the following equation which governs the large-scale (slow variable) dynamics

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

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 $\langle \vec{\nabla}_y \cdot \vec{\nabla}_x \phi^{(1)} \rangle = 0$. The convergence of ϕ^δ to $\bar{\phi}$ as $\delta \to 0$ is in L^2 [9],

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

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

Inserting equation (A-8) into (A-10) yields equation (6) with the components $\mathcal{K}^*_{jk} = \boldsymbol{\mathcal{K}}^* \vec{e}_j \cdot \vec{e}_k$ of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ given by

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

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 $\vec{\nabla}_y \chi_j$ and the *skew-symmetric* operator $\mathbf{S} = \mathbf{H} + (-\Delta_y)^{-1}\mathbf{T}$, where the inverse operation $(-\Delta_y)^{-1}$ is based on convolution with the Green's function for the Laplacian Δ_y, $\mathbf{T} = \partial_\tau \mathbf{I}$, and the $\mathbf{I}$ in this definition is to remind us that the derivative ∂_τ operates component-wise. Indeed, writing $\partial_\tau \chi_j = \vec{\nabla}_y \cdot (\Delta_y^{-1}\mathbf{T}) \vec{\nabla}_y \chi_j$, $\Delta_y \chi_j = \vec{\nabla}_y \cdot \vec{\nabla}_y \chi_j$, and $\vec{u} = \vec{\nabla}_y \cdot \mathbf{H}$ in (3), we have

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

where we have used the periodicity of χ_k and $\mathbf{H}$ to obtain the third equality. Equations (A-12) and (A-13) are equivalent to equations (8) and (9), 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 $\boldsymbol{\mathcal{K}}^*$ emerges. In Section 3, we use the analytical structure of the cell problem (A-9) to derive a resolvent representation for $\vec{\nabla}_y \chi_k$, involving an anti-symmetric integro-differential operator $\mathbf{A}$ which is related to $\mathbf{S} = \mathbf{H} - \boldsymbol{\Delta}^{-1} \partial_t \mathbf{I}$. In Section 4, we employ this representation for $\vec{\nabla}_y \chi_k$ and the spectral theorem, to provide integral representations for $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ involving a *spectral measure* associated with the operator $\mathbf{A}$ acting on a suitable Hilbert space.

A-1.3. **Symmetries and commutativity.** THIS SECTION IS UNDER CONSTRUCTION

We now show that the incompressibility of $\vec{u}$ in (2) implies that the operator $(\Delta^{-1})(\vec{u} \cdot \vec{\nabla})$ is anti-symmetric on $\mathcal{F}$ [6]. Indeed, since $\Delta = \vec{\nabla} \cdot \vec{\nabla}$ and (Δ^{-1}) is self-adjoint on $\mathcal{H}^1_{\mathcal{V}}$, for $f, h \in \mathcal{F}$ we have

$$\begin{aligned} \langle (\Delta^{-1})(\vec{u} \cdot \vec{\nabla}) f, h \rangle_1 &= \langle [\vec{\nabla}(\Delta^{-1})(\vec{u} \cdot \vec{\nabla}) f] \cdot \vec{\nabla} h \rangle \\ &= -\langle [(\vec{u} \cdot \vec{\nabla}) f] \, h \rangle \\ &= -\langle [\vec{\nabla} \cdot (\vec{u} f)] \, h \rangle \\ &= \langle f \, [(\vec{u} \cdot \vec{\nabla}) h] \rangle \\ &= \langle (\Delta^{-1}) \Delta f \, [(\vec{u} \cdot \vec{\nabla}) h] \rangle \\ &= -\langle \vec{\nabla} f \, [\vec{\nabla}(\Delta^{-1})(\vec{u} \cdot \vec{\nabla}) h] \rangle \\ &= -\langle f, (\Delta^{-1})(\vec{u} \cdot \vec{\nabla}) h \rangle_1 \end{aligned} \tag{A-14}$$

A-1.4. **Existence and Uniqueness.** THIS SECTION IS UNDER CONSTRUCTION

Before we discuss how the Hilbert space framework presented above leads to an integral representation for $\boldsymbol{\mathcal{K}}^*$, we first discuss some key differences in the theory between the cases of steady and dynamic velocity fields $\vec{u}$. These differences are reflected in the measure underlying this integral representation for $\boldsymbol{\kappa}^*$ and stem from the *unboundedness* of the operator ∂_t on the Hilbert space $\mathscr{H}_\mathcal{T}$ [31, 34]. For steady $\vec{u}$, in general, equation (13) reduces to (9) for diagonal components of the effective parameter. However, for dynamic $\vec{u}$, this is not true in general. The details are as follows. For dynamic $\vec{u}$, the operator $\boldsymbol{\sigma}$ in (12) can be written as $\boldsymbol{\sigma}=\varepsilon\mathbf{I}+\mathbf{S}$, where $\mathbf{S}=\mathbf{H}-\boldsymbol{\Delta}^{-1}\partial_t\mathbf{I}$ is skew-symmetric $\langle\mathbf{S}\vec{\xi},\vec{\zeta}\,\rangle=-\langle\vec{\xi},\mathbf{S}\vec{\zeta}\,\rangle$ for all $\vec{\xi},\vec{\zeta}\in\mathscr{F}$ such that $|\langle\partial_t\vec{\xi},\vec{\zeta}\,\rangle|,|\langle\vec{\xi},\partial_t\vec{\zeta}\,\rangle|<\infty$ (see Section A-1 for details). This property of the operator $\mathbf{S}$ implies that

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

for all such $\vec{\xi}\in\mathscr{F}$. In this dynamic setting, equation (10) does not hold for every $\vec{\xi}\in\mathscr{F}$, as the unbounded operator ∂_t is defined only on a proper (dense) subset of the Hilbert space $\mathscr{H}_\mathcal{T}$ [31], and it may be that $|\langle\partial_t\vec{\xi},\vec{\xi}\,\rangle|=\infty$. In the case of a steady velocity field we have $\mathbf{S}\equiv\mathbf{H}$ and, by equation (17) and the Cauchy Schwartz inequality, $|\langle\mathbf{S}\vec{\xi},\vec{\xi}\,\rangle|\leq\|\mathbf{H}\|\|\vec{\xi}\,\|^2<\infty$ for all $\vec{\xi}\in\mathscr{F}$, so equation (10) holds for all $\vec{\xi}\in\mathscr{F}$.

Another immediate consequence of equation (10), for steady $\vec{u}$, is the coercivity of the bilinear functional $\Phi(\vec{\xi},\vec{\zeta}\,)=\langle\boldsymbol{\sigma}\vec{\xi}\cdot\vec{\zeta}\,\rangle$ for all $\varepsilon>0$. By equation (17), this functional is also bounded in the case of steady $\vec{u}$ for all $\varepsilon<\infty$. Therefore, the Lax-Milgram theorem [22] provides the existence and uniqueness of a solution $\vec{\nabla}\chi_k\in\mathscr{F}$ satisfying the cell problem (7), or equivalently equation (12), in this time-independent case. The details are as follows.

The distributional form of equation (7), written as $\vec{\nabla}\cdot\boldsymbol{\sigma}\vec{E}_k=0$, is given by $\langle\boldsymbol{\sigma}(\vec{\nabla}\chi_k+\vec{e}_k)\cdot\vec{\nabla}\zeta\rangle=0$, where ζ is a compactly supported, infinitely differentiable function on $\mathcal{T}\otimes\mathcal{V}$, and we stress that $\vec{\nabla}\zeta$ is *curl-free*. Motivated by this, we consider the following variational problem: find $\vec{\nabla}\chi_k\in\mathscr{F}$ such that

$$\langle\boldsymbol{\sigma}(\vec{\nabla}\chi_k+\vec{e}_k)\cdot\vec{\xi}\,\rangle=0,\ \text{ for all }\vec{\xi}\in\mathscr{F}. \tag{A-16}$$

In order to directly apply the Lax-Milgram Theorem, we rewrite equation (A-16) as

$$\Phi(\vec{\nabla}\chi_k,\vec{\xi}\,)=\langle\boldsymbol{\sigma}\vec{\nabla}\chi_k\cdot\vec{\xi}\,\rangle=-\langle\boldsymbol{\sigma}\vec{e}_k\cdot\vec{\xi}\,\rangle=f(\vec{\xi}\,). \tag{A-17}$$

By equation (10) Φ is coercive, i.e.

$$\Phi(\vec{\xi},\vec{\xi}\,)=\langle[(\varepsilon\mathbf{I}+\mathbf{S})]\vec{\xi}\cdot\vec{\xi}\,\rangle=\varepsilon\|\vec{\xi}\,\|^2>0,\ \text{ for all }\vec{\xi}\in\mathscr{F} \tag{A-18}$$

such that $\|\vec{\xi}\,\|\neq0$ and $\varepsilon>0$, where $\|\cdot\|$ is the norm induced by the inner-product $\langle\cdot,\cdot\rangle$. Recall that $\mathbf{S}=\mathbf{H}$ in this time-independent case. This, equation (17), the triangle inequality, and the Cauchy-Schwartz inequality imply that Φ is also bounded for all $\varepsilon<\infty$

$$\Phi(\vec{\xi},\vec{\zeta}\,)\leq(\varepsilon+\|H\|)\|\vec{\xi}\,\|\|\vec{\zeta}\,\|<\infty,\ \text{ for all }\vec{\xi}\in\mathscr{F}. \tag{A-19}$$

For the same reasons, the linear functional $f(\vec{\xi}\,)$ in (A-17) is bounded for all $\vec{\xi}\in\mathscr{F}$. Therefore, the Lax-Milgram theorem [22] provides the existence of a unique $\vec{\nabla}\chi_k\in\mathscr{F}$ satisfying (7) in this time-independent case.

In the time-dependent case, equation (10) hence (A-18) does not hold for all $\vec{\xi}\in\mathscr{F}$. Moreover, the operator ∂_t hence $\boldsymbol{\sigma}$ is not bounded on $\mathscr{F}$ [31, 33], so (A-19) does not hold. Consequently, the Lax-Milgram theorem cannot be directly applied, and alternate techniques [13, 14] must be used to prove the existence and uniqueness of a solution $\vec{\nabla}\chi_k\in\mathscr{F}$ satisfying the cell problem (7). This discussion illustrates key differences in the analytic structure of the effective parameter problem for $\boldsymbol{\kappa}^*$, between the cases of steady and dynamic velocity fields $\vec{u}$, which stem from the unboundedness of the operator ∂_t on $\mathscr{H}_\mathcal{T}$, hence $\boldsymbol{\sigma}$ on $\mathscr{F}$. In Section 4, 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 $\boldsymbol{\kappa}^*$.

Acknowledgements.

References

[1] M. Avellaneda and A. Majda. Stieltjes integral representation and effective diffusivity bounds for turbulent transport. *Phys. Rev. Lett.*, 62:753–755, 1989.

[2] M. Avellaneda and A. Majda. An integral representation and bounds on the effective diffusivity in passive advection by laminar and turbulent flows. *Comm. Math. Phys.*, 138:339–391, 1991.

[3] M. Avellaneda and M. Vergassola. Stieltjes integral representation of effective diffusivities in time-dependent flows. *Phys. Rev. E*, 52(3):3249–3251, 1995.

[4] A. Bensoussan, J.-L. Lions, and G. Papanicolaou. *Asymptotic Analysis for Periodic Structures*. North-Holland, Amsterdam, 1978.

[5] H. Bhatia, G. Norgard, V. Pascucci, and Peer-Timo Bremer. The helmholtz-hodge decomposition-a survey. *IEEE T. Vis. Comput. Gr.*, 19(8):1386–1404, 2013.

[6] R. Bhattacharya. Multiscale diffusion processes with periodic coefficients and an application to solute transport in porous media. *Ann. Appl. Probab.*, 9(4):951–1020, 1999.

[7] L. Biferale, A. Crisanti, M. Vergassola, and A. Vulpiani. Eddy diffusivities in scalar transport. *Phys. Fluids*, 7:2725–2734, 1995.

[8] James W. Demmel. *Applied Numerical Linear Algebra*. SIAM, 1997.

[9] A. Fannjiang and G. Papanicolaou. Convection enhanced diffusion for periodic flows. *SIAM Journal on Applied Mathematics*, 54(2):333–408, 1994.

[10] A. Fannjiang and G. Papanicolaou. Convection-enhanced diffusion for random flows. *J. Stat. Phys.*, 88(5-6):1033–1076, 1997.

[11] G. B. Folland. *Introduction to Partial Differential Equations*. Princeton University Press, Princeton, NJ, 1995.

[12] G. B. Folland. *Real Analysis: Modern Techniques and Their Applications*. Wiley–Interscience, New York, NY, 1999.

[13] A. Friedman. *Partial Differential Equations*. Holt, Rinehart and Winston, 1969.

[14] A. Friedman. *Partial Differential Equations of Parabolic Type*. Dover Books on Mathematics Series. DOVER PUBN Incorporated, 2008.

[15] K. M. Golden and G. Papanicolaou. Bounds for effective parameters of heterogeneous media by analytic continuation. *Commun. Math. Phys.*, 90:473–491, 1983.

[16] P. R. Halmos. *Finite Dimensional Vector Spaces*. Van Nostrand–Reinhold, Princeton, NJ, 1958.

[17] R. A. Horn and C. R. Johnson. *Matrix Analysis*. Cambridge University Press, 1990.

[18] M. B. Isichenko and J. Kalda. Statistical topography ii. 2d transport of passive scalar. *J. Nonlinear Sci.*, 4:375–397, 1991.

[19] J. P. Keener. *Principles of applied mathematics: transformation and approximation*. Westview Press, Cambridge, MA, 2000.

[20] F. M-Denaro. On the application of the Helmholtz-Hodge decomposition in projection methods for incompressible flows with general boundary conditions. *Int. J. Numer. Meth. Fl.*, 43(1):43–69, 2003.

[21] D. McLaughlin, G. Papanicolaou, and O. Pironneau. Convection of microstructure and related problems. *SIAM J. Appl. Math.*, 45:780–797, 1985.

[22] R. C. McOwen. *Partial differential equations: methods and applications*. Prentice Hall PTR, 2003.

[23] G. W. Milton. *Theory of Composites*. Cambridge University Press, Cambridge, 2002.

[24] H. K. Moffatt. Transport effects associated with turbulence with particular attention to the influence of helicity. *Rep. Prog. Phys.*, 46(5):621–664, 1983.

[25] N. B. Murphy and K. M. Golden. The Ising model and critical behavior of transport in binary composite media. *J. Math. Phys.*, 53:063506 (25pp.), 2012.

[26] G. Papanicolaou and O. Pironeau. *On the Asymptotic Behavior of Motions in Random Flows, in Stochastic Nonlinear Systems in Physics, Chemistry, and Biology, L. Arnold and R. Lefever, eds.*, volume 8, pages 36–41. Springer, Berlin Heidelberg, 1981.

[27] G. Papanicolaou and S. Varadhan. Boundary value problems with rapidly oscillating coefficients. In *Colloquia Mathematica Societatis János Bolyai 27, Random Fields (Esztergom, Hungary 1979)*, pages 835–873. North-Holland, 1982.

[28] B. N. Parlett. *The Symmetric Eigenvalue Problem*, volume 20 of *Classics in applied mathematics*. SIAM, Philidelphia, PA, Corrected reprint of the 1980 original.

[29] G. A. Pavliotis. *Homogenization theory for advection-diffusion equations with mean flow.* PhD thesis, Rensselaer Polytechnic Institute Troy, New York, 2002.
[30] G. A. Pavliotis. Asymptotic analysis of the Green–Kubo formula. *IMA J. Appl. Math.*, 75:951–967, 2010.
[31] M. C. Reed and B. Simon. *Functional Analysis*. Academic Press, San Diego CA, 1980.
[32] H. L. Royden. *Real Analysis 3Rd Ed.* Prentice-Hall Of India Pvt. Limited, 1988.
[33] I. Stakgold. *Boundary Value Problems of Mathematical Physics: 2-Volume Set*. Classics in Applied Mathematics. SIAM, 2000.
[34] M. H. Stone. *Linear Transformations in Hilbert Space*. American Mathematical Society, Providence, RI, 1964.
[35] G. I. Taylor. Diffusion by continuous movements. *Proc. London Math. Soc.*, 2:196–211, 1921.

*Department of Mathematics, 340 Rowland Hall, University of California at Irvine, Irvine, CA 92697-3875, USA
E-mail address: nbmurphy@math.uci.edu

†Department of Mathematics, 340 Rowland Hall, University of California at Irvine, Irvine, CA 92697-3875, USA
E-mail address: jxin@math.uci.edu

⋆University of Utah, Department of Mathematics, 155 S 1400 E RM 233, Salt Lake City, UT 84112-009, USA
E-mail address: zhu@math.utah.edu

‡University of Utah, Department of Mathematics, 155 S 1400 E RM 233, Salt Lake City, UT 84112-009, USA
E-mail address: elena@math.utah.edu