Decomposing parabolic eigenvalue problem

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Abstract

A decomposition of a time periodic parabolic eigenvalue problem and an application to our effective diffusivity problem.

1 An Example

Consider the parabolic eigenvalue problem:

$$\psi_t - \Delta_x \psi + \cos(t)\, b(x)\, \psi = \lambda\, \psi, \tag{1.1}$$

subject to 2π periodic boundary conditions in x and t.

Substituting $\cos t = (e^{it} + e^{-it})/2$, and $\psi = \sum_\ell \psi_\ell(x) e^{i\ell t}$ in (1.1), we have:

$$\sum_\ell e^{i\ell t}\,(i\ell\,\psi_\ell - \Delta_x \psi_\ell) + \frac{1}{2} b(x) \sum_\ell (e^{i(\ell+1)t} + e^{i(\ell-1)t})\psi_\ell = \lambda \sum_\ell \psi_\ell e^{i\ell t},$$

or:

$$\sum_\ell e^{i\ell t}\,(i\ell\,\psi_\ell - \Delta_x \psi_\ell) + \frac{1}{2} b(x) \sum_\ell (\psi_{\ell-1} + \psi_{\ell+1})\, e^{i\ell t} = \lambda \sum_\ell \psi_\ell e^{i\ell t}.$$

Extracting the ℓ-th mode on both sides gives:

$$(-\Delta_x + i\,\ell)\,\psi_\ell + \frac{1}{2}\, b(x)\,(\psi_{\ell-1} + \psi_{\ell+1}) = \lambda\,\psi_\ell, \quad \ell \in Z, \tag{1.2}$$

which can be put in a tri-diagonal matrix acting on $[\cdots, \psi_{\ell-1}, \psi_\ell, \psi_{\ell+1}, \cdots]'$, with $b(x)/2$ on the off-diagonals, $-\Delta_x + i\,\ell$ on the diagonals.

Let us find a similar derivation for the eigenvalue problem of the advection-diffusion operator, with advection field being the time periodic cell flow:

$$\vec{u}(t, \vec{x}) = (\cos y, \cos x) + \delta \cos t\,(\sin y, \sin x) := \vec{u}_1(\vec{x}) + \delta \cos t\; \vec{u}_2(\vec{x}). \tag{1.3}$$

Question: Is it possible to carry out a similar decomposition in x and y and fully reduce the differential system like (1.2) into an algebraic system ?

1.1 An Application to our effective diffusivity problem

Consider the eigenvalue problem $A\psi_l = \imath\lambda_l\psi_l$, $\imath = \sqrt{-1}$, $\lambda_l \in \mathbb{R}$, $l = 1, 2, 3, \ldots$, 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 (1.3) above. The equation $A\psi_l = \imath\lambda_l\psi_l$ may be rewritten as

$$(\partial_t + \vec{u} \cdot \vec{\nabla})\psi_l = -\imath\lambda_l \Delta\psi_l. \tag{1.4}$$

The eigenfunctions ψ_l satisfy the following orthogonality condition

$$\langle \psi_l, \psi_i \rangle_1 = \langle \vec{\nabla}\psi_l \cdot \vec{\nabla}\psi_i \rangle = \delta_{li}, \tag{1.5}$$

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 ψ_l is $\mathcal{T}\times\mathcal{V}$ periodic, mean-zero, and $\psi_l\in\mathcal{A}(\mathcal{T})\otimes\mathcal{H}^1(\mathcal{V})$, 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 $\mathcal{F}$

$$\mathcal{F}=\{f\in\mathcal{A}(\mathcal{T})\otimes\mathcal{H}^1(\mathcal{V})\,|\,\langle f\rangle=0 \text{ and is periodic on } \mathcal{T}\times\mathcal{V}\}. \tag{1.6}$$

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

$$\psi_l(t,\vec{x})=\sum_\ell \psi_\ell^l(\vec{x})\,\mathrm{e}^{\imath\ell t}, \tag{1.7}$$

where $\psi_\ell^l\in\mathcal{H}^1(\mathcal{V})$. Write $\cos t=(\mathrm{e}^{\imath t}+\mathrm{e}^{-\imath t})/2$ and insert this and (1.7) into equation (1.4), yielding

$$\sum_\ell(\imath\ell+\vec{u}_1\cdot\vec{\nabla}+\imath\lambda_l\Delta)\psi_\ell^l(\vec{x})\mathrm{e}^{\imath\ell t}+\frac{\delta}{2}\sum_\ell(\mathrm{e}^{\imath(\ell+1)t}+\mathrm{e}^{\imath(\ell-1)t})\,\vec{u}_2\cdot\vec{\nabla}\psi_\ell^l(\vec{x})=0, \tag{1.8}$$

or:

$$\sum_\ell\left[(\imath\ell+\vec{u}_1\cdot\vec{\nabla}+\imath\lambda_l\Delta)\psi_\ell^l(\vec{x})+\frac{\delta}{2}\vec{u}_2\cdot\vec{\nabla}(\psi_{\ell-1}^l(\vec{x})+\psi_{\ell+1}^l(\vec{x}))\right]\mathrm{e}^{\imath\ell t}=0. \tag{1.9}$$

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

$$(\imath\ell+\vec{u}_1\cdot\vec{\nabla})\psi_\ell^l(\vec{x})+\frac{\delta}{2}\vec{u}_2\cdot\vec{\nabla}(\psi_{\ell-1}^l(\vec{x})+\psi_{\ell+1}^l(\vec{x}))=-\imath\lambda_l\Delta\psi_\ell^l(\vec{x}). \tag{1.10}$$

The system of partial differential equations in (1.10) 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

$$\begin{aligned}(\vec{u}_1\cdot\vec{\nabla})\psi_\ell^l(\vec{x})&=\cos y\,\partial_x\psi_\ell^l(\vec{x})+\cos x\,\partial_y\psi_\ell^l(\vec{x})\\(\vec{u}_2\cdot\vec{\nabla})\psi_\ell^l(\vec{x})&=\sin y\,\partial_x\psi_\ell^l(\vec{x})+\sin x\,\partial_y\psi_\ell^l(\vec{x})\end{aligned} \tag{1.11}$$

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

$$\psi_\ell^l(\vec{x})=\sum_{m,n}a_{\ell,m,n}^l\,\mathrm{e}^{\imath(mx+ny)} \tag{1.12}$$

Write $\cos x=(\mathrm{e}^{\imath x}+\mathrm{e}^{-\imath x})/2$ and $\sin x=(\mathrm{e}^{\imath x}-\mathrm{e}^{-\imath x})/(2\imath)$, for example, and insert this and (3.47) into equation (1.11), yielding

$$\begin{aligned}&(\vec{u}_1\cdot\vec{\nabla})\psi_\ell^l\\&\quad=\frac{1}{2}\sum_{m,n}a_{\ell,m,n}^l\left[\imath m\,\mathrm{e}^{\imath mx}(\mathrm{e}^{\imath(n+1)y}+\mathrm{e}^{\imath(n-1)y})+\imath n\,\mathrm{e}^{\imath ny}(\mathrm{e}^{\imath(m+1)x}+\mathrm{e}^{\imath(m-1)x})\right]\\&(\vec{u}_2\cdot\vec{\nabla})\psi_\ell^l\\&\quad=\frac{1}{2\imath}\sum_{m,n}a_{\ell,m,n}^l\left[\imath m\,\mathrm{e}^{\imath mx}(\mathrm{e}^{\imath(n+1)y}-\mathrm{e}^{\imath(n-1)y})+\imath n\,\mathrm{e}^{\imath ny}(\mathrm{e}^{\imath(m+1)x}-\mathrm{e}^{\imath(m-1)x})\right]\end{aligned} \tag{1.13}$$

or:

$$\begin{aligned}(\vec{u}_1\cdot\vec{\nabla})\psi_\ell^l&=\frac{\imath}{2}\sum_{m,n}[m(a_{\ell,m,n-1}^l+a_{\ell,m,n+1}^l)+n(a_{\ell,m-1,n}^l+a_{\ell,m+1,n}^l)]\mathrm{e}^{\imath(mx+ny)}\\(\vec{u}_2\cdot\vec{\nabla})\psi_\ell^l&=\frac{1}{2}\sum_{m,n}[m(a_{\ell,m,n-1}^l-a_{\ell,m,n+1}^l)+n(a_{\ell,m-1,n}^l-a_{\ell,m+1,n}^l)]\mathrm{e}^{\imath(mx+ny)}.\end{aligned} \tag{1.14}$$

We also have

$$-\Delta\psi_\ell^l = \sum_{m,n} a_{\ell,m,n}^l (m^2+n^2) \mathrm{e}^{\imath(mx+ny)} \tag{1.15}$$

By the completeness of the orthogonal set $\{\mathrm{e}^{\imath(mx+ny)}\}$, inserting equations (1.14) and (1.15) into equation (1.10) yields

$$\begin{aligned}
&\imath\ell\, a_{\ell,m,n}^l + \frac{\imath}{2}[m(a_{\ell,m,n-1}^l + a_{\ell,m,n+1}^l) + n(a_{\ell,m-1,n}^l + a_{\ell,m+1,n}^l)] \\
&\qquad + \frac{\delta}{4}[m(a_{\ell-1,m,n-1}^l - a_{\ell-1,m,n+1}^l) + n(a_{\ell-1,m-1,n}^l - a_{\ell-1,m+1,n}^l) \\
&\qquad\quad + m(a_{\ell+1,m,n-1}^l - a_{\ell+1,m,n+1}^l) + n(a_{\ell+1,m-1,n}^l - a_{\ell+1,m+1,n}^l)] \\
&\qquad = \imath\lambda_l (m^2+n^2) a_{\ell,m,n}^l,
\end{aligned} \tag{1.16}$$

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

We now discuss how the orthogonality condition $\langle\psi_l, \psi_i\rangle_1 = \delta_{li}$ in (1.5) is transformed by the Fourier expansion of the eigenfunctions $\psi_l(t,\vec{x})$. This expansion of $\psi_l(t,\vec{x})$ implies that for $\vec{\nabla}\psi_l(t,\vec{x})$ as follows

$$\psi_l(t,\vec{x}) = \sum_{\ell,m,n} a_{\ell,m,n}^l \mathrm{e}^{\imath(\ell t+mx+ny)} \Rightarrow \vec{\nabla}\psi_l(t,\vec{x}) = \sum_{\ell,m,n} a_{\ell,m,n}^l\,(m,n)\,\mathrm{e}^{\imath(\ell t+mx+ny)}. \tag{1.17}$$

Recall the orthogonality relation

$$\left\langle \mathrm{e}^{\imath(\ell t+mx+ny)},\, \mathrm{e}^{\imath(\ell' t+m'x+n'y)} \right\rangle_2 = (2\pi)^3 \delta_{\ell,\ell'}\delta_{m,m'}\delta_{n,n'}, \tag{1.18}$$

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 (1.5) is transformed to

$$\delta_{li} = \langle\vec{\nabla}\psi_l \cdot \vec{\nabla}\psi_i\rangle = \sum_{\ell,m,n} (m^2+n^2)\,\overline{a_{\ell,m,n}^l}\, a_{\ell,m,n}^i \tag{1.19}$$

Recall that $\sum_i i^{-p}$ converges for all $p > 1$. From this and equation (1.19) we see that the square modulus of the Fourier coefficients $a_{0,m,n}^l$ must have the asymptotic behavior $|a_{0,m,n}^l|^2 \sim o((m^2+n^2)^{-3/2})$ as $m, n \to \pm\infty$. Since $\psi_l(\cdot,\vec{x}) \in \mathcal{A}(\mathcal{T})$, i.e. $\partial_t\psi_l(\cdot,\vec{x}) \in L^2(\mathcal{T})$, we also have $|a_{\ell,m,n}^l|^2 \sim o(\ell^{-3})$ as $\ell \to \pm\infty$. Since $\partial_t\vec{\nabla}\psi_l \in L^2(\mathcal{T}\times\mathcal{V})$ we may generalize both of these statements by the following

$$|a_{\ell,m,n}^l|^2 \sim o(\ell^{-3}(m^2+n^2)^{-3/2}), \text{ as } \ell, m, n \to \pm\infty. \tag{1.20}$$

We now use the special nature of the velocity field in (1.3) and the Fourier expansion of the eigenfunctions in (1.17) to show that the Radon–Stieltjes integral representation for the symmetric $\boldsymbol{\kappa}^*$ and anti-symmetric $\boldsymbol{\alpha}^*$ parts of the effective diffusivity tensor $\boldsymbol{\mathcal{K}}^*$ depend only on the Fourier coefficients $a_{\ell,m,n}^l$ for $\ell, m, n \in \{-1, 0, 1\}$. Recall that the Hilbert space $\mathcal{H}$ underlying this problem is

$$\mathcal{H} = \{f \in L^2(\mathcal{T}) \otimes \mathcal{H}^1(\mathcal{V}) \,|\, \langle f\rangle = 0 \text{ and is periodic on } \mathcal{T}\times\mathcal{V}\}, \tag{1.21}$$

with A maximal normal, i.e. $\imath A$ self-adjoint, on $\mathcal{F} \subset \mathcal{H}$ defined in (1.6). Since the eigenfunctions ψ_l and ψ_i of A associated with distinct eigenvalues, $\lambda_l \neq \lambda_i$, are orthonormal, $\langle\psi_l,\psi_i\rangle_1 = \langle\vec{\nabla}\psi_l\cdot\vec{\nabla}\psi_i\rangle = \delta_{li}$, the span of all eigenfunctions constitutes a closed linear manifold $\mathcal{E}$ in $\mathcal{F}$. Let $\mathcal{E}^\perp$ be its (closed) orthogonal complement in $\mathcal{H}$ so that [Stone]

$$\mathcal{H} = \mathcal{E} \oplus \mathcal{E}^\perp. \tag{1.22}$$

Recall the cell problem

$$(\varepsilon + A)\chi_j = g_j, \quad g_j = (-\Delta)^{-1}u_j, \tag{1.23}$$

where u_j is the j^{th} component of the velocity field $\vec{u}$. Since $\chi_j, g_j \in \mathcal{F}$ and $\mathcal{F} \subset \mathcal{E} \oplus \mathcal{E}^{\perp}$ they have the following representations

$$\chi_j = \sum_l \langle \psi_l, \chi_j \rangle_1 \, \psi_l + \chi_j^{\perp}, \quad g_j = \sum_l \langle \psi_l, g_j \rangle_1 \, \psi_l + g_j^{\perp}, \tag{1.24}$$

where $\psi_l \in \mathcal{E}$ and $\chi_j^{\perp}, g_j^{\perp} \in \mathcal{E}^{\perp}$. Using $A\psi_l = \imath\lambda_l\psi_l$, $\lambda_l \in \mathbb{R}$, and the orthonormality of the set $\{\psi_l\}$, inserting (1.24) into the cell problem (1.23) yields

$$\sum_l [(\varepsilon - \imath\lambda_l)\langle \psi_l, \chi_j \rangle_1 - \langle \psi_l, g_j \rangle_1]\psi_l + (\varepsilon + A)\chi_j^{\perp} - g_j^{\perp} = 0. \tag{1.25}$$

By the orthonormality of the set $\{\psi_l\}$ and since $\langle A\chi_j^{\perp}, \psi_l \rangle_1 = -\langle \chi_j^{\perp}, A\psi_l \rangle_1 = -\imath\lambda_l \langle \chi_j^{\perp}, \psi_l \rangle_1 = 0$, taking the inner-product of both sides of (1.25) with ψ_l yields

$$\langle \psi_l, \chi_j \rangle_1 = \frac{\langle \psi_l, g_j \rangle_1}{(\varepsilon - \imath\lambda_l)}, \quad 0 < \varepsilon < \infty. \tag{1.26}$$

Recall that the components κ^*_{jk} and α^*_{jk} of $\boldsymbol{\kappa}^*$ and $\boldsymbol{\alpha}^*$ are given by

$$\kappa^*_{jk} = \varepsilon(\delta_{jk} + \langle \chi_j, \chi_k \rangle_1), \quad \alpha^*_{jk} = \langle A\chi_j, \chi_k \rangle_1. \tag{1.27}$$

From equations (1.24) and (1.26) and the orthonormality of the set $\{\psi_l\}$, we have

$$\begin{aligned} \langle \chi_j, \chi_k \rangle_1 - \langle \chi_j^{\perp}, \chi_k^{\perp} \rangle_1 &= \sum_l \overline{\langle \psi_l, \chi_j \rangle_1} \langle \psi_l, \chi_k \rangle_1 = \sum_l \frac{\overline{\langle \psi_l, g_j \rangle_1} \langle \psi_l, g_k \rangle_1}{\varepsilon^2 + \lambda_l^2} \\ \langle A\chi_j, \chi_k \rangle_1 - \langle A\chi_j^{\perp}, \chi_k^{\perp} \rangle_1 &= \sum_l (-\imath\lambda_l) \overline{\langle \psi_l, \chi_j \rangle_1} \langle \psi_l, \chi_k \rangle_1 = \sum_l \frac{(-\imath\lambda_l) \overline{\langle \psi_l, g_j \rangle_1} \langle \psi_l, g_k \rangle_1}{\varepsilon^2 + \lambda_l^2} \end{aligned} \tag{1.28}$$

The right hand sides of the formulas in equation (1.28) 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 with respect to *continuous* measures, and provides the standard decomposition of the *spectral measure* into its discrete and continuous components, in the general setting [Stone].

We now show that the special nature of the velocity field in (1.3) and the Fourier expansion of the eigenfunctions ψ_l in (1.17) allow the spectral weights $\langle \psi_l, g_j \rangle$ in equation (1.28) to be given in terms of the Fourier coefficients $a^l_{\ell,m,n}$ for the reduced index set $\ell, m, n \in \{-1, 0, 1\}$. First note that, since $u_j(t, \cdot) \in \mathcal{H}^1(\mathcal{V}) \subset L^2(\mathcal{V})$,

$$\langle \psi_l, g_j \rangle_1 = \langle \vec{\nabla}\psi_l \cdot \vec{\nabla}(-\Delta)^{-1}u_j \rangle = \langle \psi_l, (-\Delta)(-\Delta)^{-1}u_j \rangle_2 = \langle \psi_l, u_j \rangle_2. \tag{1.29}$$

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 (1.3) we have that

$$\begin{aligned} u_1(t, x, y) &= \cos y + \cos t \sin y \\ &= \frac{1}{2}\left(\mathrm{e}^{\imath y} + \mathrm{e}^{-\imath y}\right) + \frac{1}{4\imath}\left(\mathrm{e}^{\imath t} + \mathrm{e}^{-\imath t}\right)(\mathrm{e}^{\imath y} - \mathrm{e}^{-\imath y}) \\ &= \frac{1}{2}\left(\mathrm{e}^{\imath y} + \mathrm{e}^{-\imath y}\right) + \frac{1}{4\imath}\left(\mathrm{e}^{\imath(t+y)} - \mathrm{e}^{\imath(t-y)} + \mathrm{e}^{\imath(-t+y)} - \mathrm{e}^{\imath(-t-y)}\right), \end{aligned} \tag{1.30}$$

and $u_2(t, x, y) = u_1(t, y, x)$. This, equation (1.29), and the orthogonality relation in (1.18) imply that

$$\begin{aligned} \langle \psi_l, g_1 \rangle_1 &= \frac{1}{2}\left(a^l_{0,0,1} + a^l_{0,0,-1}\right) + \frac{1}{4\imath}\left(a^l_{1,0,1} - a^l_{1,0,-1} + a^l_{-1,0,1} - a^l_{-1,0,-1}\right) \\ \langle \psi_l, g_2 \rangle_1 &= \frac{1}{2}\left(a^l_{0,1,0} + a^l_{0,-1,0}\right) + \frac{1}{4\imath}\left(a^l_{1,1,0} - a^l_{1,-1,0} + a^l_{-1,1,0} - a^l_{-1,-1,0}\right) \end{aligned} \tag{1.31}$$

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 (1.4) becomes

$$\vec{\nabla} \cdot \mathbf{H}_1 \vec{\nabla} \psi = \lambda \Delta \psi. \tag{1.32}$$

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.

1.1.1 Matrix representations of the eigenvalue problem

In the *time-independent case*, where $\delta = 0$ in the velocity field of equation (1.3), the system of equations in (1.16) corresponding to the eigenvalue problem becomes

$$m(a_{m,n-1} + a_{m,n+1}) + n(a_{m-1,n} + a_{m+1,n}) = 2\lambda(m^2 + n^2)a_{m,n}, \quad m, n \in \mathbb{Z}, \tag{1.33}$$

where, for simplicity, we have dropped the super-script and sub-script, and have written $a_{m,n} = a^{\,l}_{m,n}$ and $\lambda = \lambda_l$. When the indices in equation (1.33) are restricted to be finite, $-M \leq m, n \leq M$ say, and suitable boundary conditions are imposed, it can be written in matrix form

$$B\vec{a}_l = 2\lambda_l C \vec{a}_l, \tag{1.34}$$

where B and C are $(2M+1)^2 \times (2M+1)^2$ symmetric matrices and $l = 1, \ldots, (2M+1)^2$. More specifically, B is real-symmetric and C is real-diagonal positive-semi-definite. Equation (1.34) is a generalized eigenvalue problem. Since B and C are symmetric matrices, the generalized eigenvalues are real $\lambda_l \in \mathbb{R}$ and the eigen-vectors $\vec{a}_l$ – consisting of the Fourier coefficients for ψ_l – satisfy the orthogonality condition

$$\vec{a}_j^{\,T} C \vec{a}_k = \delta_{jk}. \tag{1.35}$$

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 $\delta \neq 0$ in the velocity field of equation (1.3), slightly manipulating equation (1.16) yields

$$\begin{aligned}
4\ell\, a_{\ell,m,n} &+ 2[m(a_{\ell,m,n-1} + a_{\ell,m,n+1}) + n(a_{\ell,m-1,n} + a_{\ell,m+1,n})] \\
&\quad -\imath\delta[m(a_{\ell-1,m,n-1} - a_{\ell-1,m,n+1} + a_{\ell+1,m,n-1} - a_{\ell+1,m,n+1}) \\
&\qquad +n(a_{\ell-1,m-1,n} - a_{\ell-1,m+1,n} + a_{\ell+1,m-1,n} - a_{\ell+1,m+1,n})] \\
&= 4\lambda(m^2 + n^2)a_{\ell,m,n}.
\end{aligned} \tag{1.36}$$

By restricting the indices, $-M \leq l, m, n \leq M$, in equation (1.36) and imposing suitable boundary conditions, it can also be written as the generalized eigenvalue problem of equations (1.34) and (1.35), 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.

2 Three-Dim Steady Cellular Flows

The 3 dimensional (3D) steady cellular flows are:

$$B = (\Phi_x(x,y)W'(z), \Phi_y(x,y)W'(z), k\Phi(x,y)W(z)), \tag{2.37}$$

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

A special case is $k = 2$, then

$$\vec{u}(x, y, z) = (-\sin x\, \cos y\, \cos z, -\cos x\, \sin y\, \cos z, 2\cos x\, \cos y\, \sin z). \tag{2.38}$$

We now derive a system of algebraic equations, analogous to that of equation (1.16), corresponding to the velocity field $\vec{u}$ displayed in (2.38). The steady state eigenvalue problem of equation (1.4) is given by

$$\vec{u} \cdot \vec{\nabla}\psi_l = -\imath\lambda_l \Delta\psi_l. \tag{2.39}$$

The analog of equation (1.11) is

$$(\vec{u} \cdot \vec{\nabla})\psi_l(\vec{x}) = -\sin x\, \cos y\, \cos z\, \partial_x\psi_l(\vec{x}) - \cos x\, \sin y\, \cos z\, \partial_y\psi_l(\vec{x}) + 2\cos x\, \cos y\, \sin z\, \partial_z\psi_l(\vec{x}). \tag{2.40}$$

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

$$\psi_l(\vec{x}) = \sum_{\ell,m,n} a^l_{\ell,m,n} \mathrm{e}^{\imath(\ell x+my+nz)}. \tag{2.41}$$

Using the identities

$$\begin{aligned}
u_1(\vec{x}) &= -\sin x\, \cos y\, \cos z = -\frac{1}{4}(+\sin(x-y-z) + \sin(x-y+z) + \sin(x+y-z) + \sin(x+y+z)) \\
u_2(\vec{x}) &= -\cos x\, \sin y\, \cos z = \frac{1}{4}(+\sin(x-y-z) + \sin(x-y+z) - \sin(x+y-z) - \sin(x+y+z)) \\
u_3(\vec{x}) &= 2\cos x\, \cos y\, \sin z = \frac{1}{2}(-\sin(x-y-z) + \sin(x-y+z) - \sin(x+y-z) + \sin(x+y+z)),
\end{aligned} \tag{2.42}$$

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 (1.16) for the velocity field in (2.38) is given by

$$\begin{aligned}
&-\frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m+1,n+1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m-1,n-1} - \frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m+1,n-1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m-1,n+1} \\
&-\frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m-1,n+1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m+1,n-1} - \frac{\imath(\ell-1)}{8\imath}a_{\ell-1,m-1,n-1} + \frac{\imath(\ell+1)}{8\imath}a_{\ell+1,m+1,n+1} \\
&\frac{\imath(m+1)}{8\imath}a_{\ell-1,m+1,n+1} - \frac{\imath(m-1)}{8\imath}a_{\ell+1,m-1,n-1} + \frac{\imath(m+1)}{8\imath}a_{\ell-1,m+1,n-1} - \frac{\imath(m-1)}{8\imath}a_{\ell+1,m-1,n+1} \\
&-\frac{\imath(m-1)}{8\imath}a_{\ell-1,m-1,n+1} + \frac{\imath(m+1)}{8\imath}a_{\ell+1,m+1,n-1} - \frac{\imath(m-1)}{8\imath}a_{\ell-1,m-1,n-1} + \frac{\imath(m+1)}{8\imath}a_{\ell+1,m+1,n+1} \\
&-\frac{\imath(n+1)}{4\imath}a_{\ell-1,m+1,n+1} + \frac{\imath(n-1)}{4\imath}a_{\ell+1,m-1,n-1} + \frac{\imath(n-1)}{4\imath}a_{\ell-1,m+1,n-1} - \frac{\imath(n+1)}{4\imath}a_{\ell+1,m-1,n+1} \\
&-\frac{\imath(n+1)}{4\imath}a_{\ell-1,m-1,n+1} + \frac{\imath(n-1)}{4\imath}a_{\ell+1,m+1,n-1} + \frac{\imath(n-1)}{4\imath}a_{\ell-1,m-1,n-1} - \frac{\imath(n+1)}{4\imath}a_{\ell+1,m+1,n+1} \\
&=\imath\lambda_l(m^2+n^2)a_{\ell,m,n},
\end{aligned} \tag{2.43}$$

where we have suppressed the super-script notation and written $a^l_{\ell,m,n} = a_{\ell,m,n}$. Simplifying equation (2.43) yields

$$\begin{aligned}
&\imath((\ell-1) - (m+1) + 2(n+1))a_{\ell-1,m+1,n+1} + \imath(-(\ell+1) + (m-1) - 2(n-1))a_{\ell+1,m-1,n-1} \\
&+\imath((\ell-1) - (m+1) - 2(n-1))a_{\ell-1,m+1,n-1} + \imath(-(\ell+1) + (m-1) + 2(n+1))a_{\ell+1,m-1,n+1} \\
&+\imath((\ell-1) + (m-1) + 2(n+1))a_{\ell-1,m-1,n+1} + \imath(-(\ell+1) - (m+1) - 2(n-1))a_{\ell+1,m+1,n-1} \\
&+\imath((\ell-1) + (m-1) - 2(n-1))a_{\ell-1,m-1,n-1} + \imath(-(\ell+1) - (m+1) + 2(n+1))a_{\ell+1,m+1,n+1} \\
&=8\lambda_l(m^2+n^2)a_{\ell,m,n},
\end{aligned} \tag{2.44}$$

From equations (1.29) and (2.42), one can see that the analogue of equation (1.31) is given by

$$
\begin{aligned}
\langle \psi_l, g_1\rangle_1 &= -\frac{1}{8\imath}\left(+(a_{1,-1,-1}-a_{-1,1,1}) + (a_{1,-1,1}-a_{-1,1,-1}) + (a_{1,1,-1}-a_{-1,-1,1}) + (a_{1,1,1}-a_{-1,-1,-1})\right)\\
\langle \psi_l, g_2\rangle_1 &= \frac{1}{8\imath}\left(+(a_{1,-1,-1}-a_{-1,1,1}) + (a_{1,-1,1}-a_{-1,1,-1}) - (a_{1,1,-1}-a_{-1,-1,1}) - (a_{1,1,1}-a_{-1,-1,-1})\right)\\
\langle \psi_l, g_3\rangle_1 &= \frac{1}{4\imath}\left(-(a_{1,-1,-1}-a_{-1,1,1}) + (a_{1,-1,1}-a_{-1,1,-1}) - (a_{1,1,-1}-a_{-1,-1,1}) + (a_{1,1,1}-a_{-1,-1,-1})\right)
\end{aligned}
\tag{2.45}
$$

By restricting the indices, $-M \le l, m, n \le M$, in equation (2.44) and imposing suitable boundary conditions, it can also be written as the generalized eigenvalue problem of equations (1.34) and (1.35), 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.

3 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 (1.23), $(\varepsilon + A)\chi_j = g_j$, which involves the function $\chi_j(t,\vec{x})$ which is a member of the function space $\mathcal{F}$ defined in equation (1.6), $\chi_j \in \mathcal{F}$, 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

$$
(\partial_t + \vec{u}\cdot\vec{\nabla} - \varepsilon\Delta)\chi_j(t,\vec{x}) = u_j(t,\vec{x}) \tag{3.46}
$$

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

$$
\chi_j(t,\vec{x}) = \sum_{m,n} b^j_{m,n}(t)\, e^{\imath(mx+ny)}, \quad b^j_{m,n}(0) = b^j_{m,n}(2\pi) \tag{3.47}
$$

Inserting this into equation (3.46) yields

$$
\sum_{m,n} e^{\imath(mx+ny)}[\partial_t + \imath m u_1 + \imath n u_2 + \varepsilon(m^2+n^2)]b^j_{m,n} = u_j \tag{3.48}
$$

Consider the velocity field $\vec{u} = (u_1, u_2)$ defined in equation (1.3), 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 (1.13) and (1.14), equation (3.48) can be written as

$$
\begin{aligned}
\sum_{m,n} e^{\imath(mx+ny)}[\partial_t b^1_{m,n} &+ \frac{\imath}{2}(m(b^1_{m,n-1} + b^1_{m,n+1}) + n(b^1_{m-1,n} + b^1_{m+1,n}))\\
&+ \frac{\delta\cos t}{2}(m(b^1_{m,n-1} - b^1_{m,n+1}) + n(b^1_{m-1,n} - b^1_{m+1,n})) + \varepsilon(m^2+n^2)b^1_{m,n}\\
&- \frac{1}{2}\delta_{0,m}(\delta_{1,n} + \delta_{-1,n}) - \frac{\delta\cos t}{2\imath}\delta_{0,m}(\delta_{1,n} - \delta_{-1,n})] = 0.
\end{aligned}
\tag{3.49}
$$

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 (3.49), $l = -1, 0, 1$, where $\delta_{l,m}$ is the Kronecker delta. By the completeness of the orthogonal set $\{e^{\imath(mx+ny)}\}$ and equation (3.49), we have that the cell problem in (3.46) is equivalent to the following two (infinite) linear systems of coupled ordinary differential equations (ODE's)

$$\begin{aligned}
\partial_t b^1_{m,n} &+ \frac{\imath}{2}(m(b^1_{m,n-1}+b^1_{m,n+1})+n(b^1_{m-1,n}+b^1_{m+1,n})) \\
&+ \frac{\delta\cos t}{2}(m(b^1_{m,n-1}-b^1_{m,n+1})+n(b^1_{m-1,n}-b^1_{m+1,n}))+\varepsilon(m^2+n^2)b^1_{m,n} \\
&= \frac{1}{2}\delta_{0,m}(\delta_{1,n}+\delta_{-1,n})+\frac{\delta\cos t}{2\imath}\delta_{0,m}(\delta_{1,n}-\delta_{-1,n}), \\
\partial_t b^2_{m,n} &+ \frac{\imath}{2}(m(b^2_{m,n-1}+b^2_{m,n+1})+n(b^2_{m-1,n}+b^2_{m+1,n})) \\
&+ \frac{\delta\cos t}{2}(m(b^2_{m,n-1}-b^2_{m,n+1})+n(b^2_{m-1,n}-b^2_{m+1,n}))+\varepsilon(m^2+n^2)b^2_{m,n} \\
&= \frac{1}{2}\delta_{0,n}(\delta_{1,m}+\delta_{-1,m})+\frac{\delta\cos t}{2\imath}\delta_{0,n}(\delta_{1,m}-\delta_{-1,m}),
\end{aligned} \tag{3.50}$$

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 (3.50) 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 (1.3) is time-independent. In this case, equation (3.50) reduces to the following linear, algebraic system

$$\begin{aligned}
\frac{\imath}{2}(m(b^1_{m,n-1}+b^1_{m,n+1})+n(b^1_{m-1,n}+b^1_{m+1,n}))+\varepsilon(m^2+n^2)b^1_{m,n} &= \frac{1}{2}\delta_{0,m}(\delta_{1,n}+\delta_{-1,n}) \\
\frac{\imath}{2}(m(b^2_{m,n-1}+b^2_{m,n+1})+n(b^2_{m-1,n}+b^2_{m+1,n}))+\varepsilon(m^2+n^2)b^2_{m,n} &= \frac{1}{2}\delta_{0,n}(\delta_{1,m}+\delta_{-1,m}).
\end{aligned} \tag{3.51}$$

When the indices of equation (3.51) 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

$$(B+\varepsilon C)\vec{b}^{\,j}=\vec{\xi}^{\,j} \tag{3.52}$$

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 (1.27). 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 (1.18), (1.19), and (3.47) we have

$$\langle\chi_j,\chi_k\rangle_1=\sum_{m,n}(m^2+n^2)\,\langle\overline{b^j_{m,n}}\,b^k_{m,n}\rangle_t, \tag{3.53}$$

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 (1.29) 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 (3.49) we have

$$\begin{aligned}
\langle A\chi_j,\chi_k\rangle_1=\sum_{m,n}\langle\overline{\gamma^{\delta,j}_{m,n}}\,b^k_{m,n}\rangle_t,\quad \gamma^{\delta,j}_{m,n} &= \partial_t b^j_{m,n}+\frac{\imath}{2}(m(b^j_{m,n-1}+b^j_{m,n+1})+n(b^j_{m-1,n}+b^j_{m+1,n})) \\
&+ \frac{\delta\cos t}{2}(m(b^j_{m,n-1}-b^j_{m,n+1})+n(b^j_{m-1,n}-b^j_{m+1,n})).
\end{aligned} \tag{3.54}$$

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 $\gamma^{\delta,j}_{m,n}=(m(b^j_{m,n-1}+b^j_{m,n+1})+n(b^j_{m-1,n}+b^j_{m+1,n}))/(-2\imath)$.

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