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Dispersion in the large-deviation regime. Part II: cellular flow at large Péclet number

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A standard model for the study of scalar dispersion through the combined effect of advec-9 tion and molecular diffusion is a two-dimensional periodic flow with closed streamlines 10 inside periodic cells. Over long time scales, the dispersion of a scalar released in this flow 11 can be characterised by an effective diffusivity that is a factor $Pe^{1/2}$ larger than molec-12 ular diffusivity when the Péclet number Pe is large. Here we provide a more complete 13 description of dispersion in this regime by applying the large-deviation theory developed 14 in Part I of this paper. Specifically, we derive approximations to the rate function gov-15 erning the scalar concentration at large time t by carrying out an asymptotic analysis of 16 the relevant family of eigenvalue problems. 17

We identify two asymptotic regimes and, for each, make predictions for the rate func-18 tion and spatial structure of the scalar. Regime I applies to distances $|\mathbf{x}|$ from the scalar 19 release point that satisfy $|\mathbf{x}| = O(\mathrm{Pe}^{1/4}t)$. The concentration in this regime is isotropic at 20 large scales, is uniform along streamlines within each cell, and varies rapidly in boundary 21 layers surrounding the separatrices between adjacent cells. The results of homogenisation 22 theory, yielding the $O(\text{Pe}^{1/2})$ effective diffusivity, are recovered from our analysis in the 23 limit $|\mathbf{x}| \ll \text{Pe}^{1/4}t$. Regime II applies when $|\mathbf{x}| = O(\text{Pe}t/\log\text{Pe})$ and is characterised 24 by an anisotropic concentration distribution that is localised around the separatrices. A 25 novel feature of this regime is the crucial role played by the dynamics near the hyper-26 bolic stagnation points. A consequence is that in part of the regime the dispersion can 27 be interpreted as resulting from a random walk on the lattice of stagnation points. The 28 29 two regimes overlap so that our asymptotic results describe the scalar concentration over a large range of distances $|\mathbf{x}|$. They are verified against numerical solutions of the family 30 of eigenvalue problems yielding the rate function. 31

32 1. Introduction

The transport and mixing of constituents by fluid flows is a classical problem in fluid 33 dynamics, motivated by a broad range of industrial and environmental applications. One 34 35 of the main strands of the research on this problem, e.g. reviewed in Majda & Kramer (1999), examines how the interaction between advection and molecular diffusion leads to 36 enhanced transport and mixing. The dispersion resulting from advection and molecular 37 diffusion gives, in the long-time limit, both linearly increasing variance of particle posi-38 tions and Gaussian concentration distributions and can therefore be quantified by means 39 of an effective diffusivity (typically much increased compared to the molecular value). 40 Several approaches—including homogenisation—are available to calculate this effective 41

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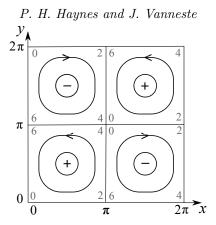


FIGURE 1. Schematic of the streamlines in single periodic cell for the flow with streamfunction (2.2). The quarter-cells with anticlockwise (clockwise) circulation are denoted by the +(-) signs. The value of the coordinate σ used in the boundary-layer analyses of §§3.2 and 4 is indicated at the corner of each quarter-cell by the grey number.

diffusivity and, in simple examples at least, they yield instructive closed-form results
(Majda & Kramer 1999). Classical examples of this type are shear flows, originally considered by Taylor (1953), and the cellular flow on which the present paper focuses. The

45 cellular flow is a two-dimensional periodic incompressible flow, with streamfunction

$$\psi = -Ua\sin(x/a)\sin(y/a),\tag{1.1}$$

where U is the maximum flow speed and $2\pi a$ is the cell period. This flow consists of a 46 doubly infinite array of periodic cells in which the fluid is rotating alternatively clock-47 wise and anti-clockwise as sketched in Fig. 1. It was introduced in studies of kinematic 48 49 dynamos (Childress 1979) and has since become a benchmark for work on advectiondiffusion (e.g. Moffatt 1983). The enhancement of dispersion by this flow (over that which 50 results from molecular diffusion alone) is encapsulated by the results of Soward (1987), 51 Shraiman (1987) and Rosenbluth et al. (1987) showing that the effective diffusivity in 52 this case scales like $\operatorname{Pe}^{1/2}$ as $\operatorname{Pe} \to \infty$. Here 53

$$Pe = Ua/\kappa, \tag{1.2}$$

with κ the molecular diffusivity, is the Péclet number, which measures the relative strength of advection and diffusion in the flow. Several other explicit results are also available for this flow, see Majda & Kramer (1999) and references therein.

When applied to initial-value problems, which typically involve a passive scalar released 57 initially in a small region, the characterisation of dispersion by a single effective diffusivity 58 relies on an implicit assumption: the distances $|\mathbf{x}|$ between points of interest and the 59 scalar-release region are assumed to be moderately large, specifically to be $O(t^{1/2})$ for 60 large times t. For larger distances, the approximation by a diffusive. Gaussian process is 61 invalid. In a companion paper (Haynes & Vanneste 2014, hereafter referred to as Part 62 I) we show that the scalar distribution at such distances can nonetheless by described 63 analytically, using the theory of large deviations. Part I provides a general formulation for 64 the theory of large deviations relevant to dispersion problems and applies it to shear flows 65 and to periodic flows including the cellular flow (1.1). The results presented there for the 66 cellular flow are largely numerical although asymptotic expressions are obtained in the 67 regime $Pe \ll 1$ corresponding to weak advection. In the present paper we obtain detailed 68 asymptotic results for the opposite, and arguably more physically interesting, regime 69 $Pe \gg 1$ corresponding to weak diffusion. In this limit, diffusion acts as a small, singular 70

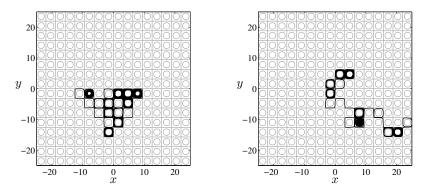


FIGURE 2. Examples of particle trajectories for Pe = 1000. The black lines show the trajectories $\boldsymbol{x}(t)$ for $0 \le t \le 2000$ of two particles initially released at the origin for two different realisations of the Brownian motion. The grey lines indicate the streamlines $\psi = 0$ (separatrices) and $\psi = \pm 1/2$.

⁷¹ perturbation to advection: in the complete absence of diffusion, there is no large-scale ⁷² transport since particle trajectories are confined to closed streamlines inside quarter cells ⁷³ (see Figure 1). A weak diffusion makes it possible for particles to migrate from streamline ⁷⁴ to streamline and, when crossing the separatrices, from cell to cell, leading to large-scale ⁷⁵ transport. The importance of the separatrices is reflected in the asymptotic analysis ⁷⁶ which largely consists of a boundary-layer treatment of an $O(\text{Pe}^{-1/2})$ region surrounding ⁷⁷ them.

Specifically, we identify and study two asymptotic regimes, characterised by differ-78 ent scalings of $|\mathbf{x}|/t$ relative to Pe and leading to different asymptotic reductions. The 79 boundary-layer analysis in the first regime turns out to be same as that appearing in 80 the computation of the $O(\text{Pe}^{1/2})$ effective diffusivity (Childress 1979; Soward 1987), even 81 though the regime applies over a broader range of $|\mathbf{x}|/t$ and captures non-diffusive effects. 82 The boundary-layer analysis in the second case is novel. It requires a careful treatment 83 of the regions around the stagnation points, leading to a logarithmic dependence of the 84 results on Pe. Note that in both cases the asymptotic analysis is formal: we make no 85 attempt at bounding error terms. Instead, we check our asymptotic predictions against 86 numerical solutions of the eigenvalue problem determining the scalar concentration in 87 the large-deviation regime, and we find excellent agreement. 88

Before entering the intricacies of this asymptotic analysis, however, it is useful to have 89 in mind a physical picture of dispersion in the cellular flow at high Pe. Figure 5 of Part 90 I illustrates the dispersion by displaying the evolution of the concentration of a passive 91 scalar released in the central cell. It indicates a transition, moving away from the release 92 region, between cells that have near-uniform concentrations near the centre and cells 93 that are depleted at larger distances, with non-zero concentration essentially confined to 94 the neighbourhood of the separatrices. The asymptotic analysis presented in this paper 95 captures this transition and provides the analytic form of the concentration distribution 96 over a broad range of distances. An alternative view of the problem considers independent 97 particles released in the flow (1.1) and experiencing different realisations of the Brownian 98 motion associated with diffusion. In this view, the (normalised) scalar concentration is 99 interpreted as the particle-position probability distribution function. The motion of single 100 particles is illustrated in Figure 2 showing two trajectory realisations. As expected, most 101 of the time particles are trapped within quarter cells for long times; as the right panel 102 suggests, however, large excursions are possible when the Brownian motion is such that 103

the particle remains close to the separatrix for some time. The statistics at large distances from the release point are then controlled by rare realisations of the Brownian motion for which the particle only rarely visits the cell interiors. The large-deviation theory we employ is the probabilistic tool required to capture the statistics of these rare realisations.

108 2. Formulation

We examine the dispersion of a passive scalar in the cellular flow with streamfunction (1.1). The concentration $C(\boldsymbol{x},t)$ of a passive scalar released in this flow is governed by the advection-diffusion equation. Using *a* as reference length and the diffusive time scale a^2/κ as reference time, this equation takes the non-dimensional form

$$\partial_t C + \operatorname{Pe} \boldsymbol{u} \cdot \nabla C = \nabla^2 C, \qquad (2.1)$$

113 where $\boldsymbol{u} = (-\partial_{\boldsymbol{u}}\psi, \partial_{\boldsymbol{x}}\psi)$ and

$$\psi = -\sin x \sin y \tag{2.2}$$

are the dimensionless velocity and streamfunction. We consider the initial-value problem with initial condition $C(\boldsymbol{x}, 0) = \delta(\boldsymbol{x})$ so that $C(\boldsymbol{x}, t)$ can interpreted as a particle-position probability density function for a particle released at the origin.

In Part I, we show that the concentration for $t \gg 1$ takes the large-deviation form

$$C(\boldsymbol{x},t) \sim t^{-1}\phi(\boldsymbol{x},\boldsymbol{\xi})e^{-tg(\boldsymbol{\xi})}, \text{ where } \boldsymbol{\xi} = \boldsymbol{x}/t.$$
 (2.3)

The Cramér or rate function $q(\boldsymbol{\xi})$ which appears in (2.3) controls the dispersion for 118 x = O(t) and is our main object of interest. It can be determined as the Legendre 119 transform of the dual function f(q), identified as t^{-1} times the cumulant generating 120 function $\log \mathbb{E} e^{q \cdot X}$ for the position X of particles advected and diffused in the flow, 121 where \mathbb{E} denotes expectation over the Brownian motion associated with diffusion. The 122 relationship between $g(\boldsymbol{\xi})$ and $f(\boldsymbol{q})$ follows from the Ellis-Gärtner theorem, a key result 123 of large-deviation theory (e.g. Ellis 1995; Dembo & Zeitouni 1998; den Hollander 2000; 124 Touchette 2009). In turn, f(q) is found as the principal eigenvalue of the eigenvalue 125 problem 126

$$\nabla^2 \phi - (\operatorname{Pe} \boldsymbol{u} + 2\boldsymbol{q}) \cdot \nabla \phi + (\operatorname{Pe} \boldsymbol{u} \cdot \boldsymbol{q} + |\boldsymbol{q}|^2) \phi = f(\boldsymbol{q})\phi, \qquad (2.4)$$

where $q = (q_1, q_2)$ is regarded as a parameter and $\phi(x, q)$ is the eigenfunction which satisfies periodic boundary conditions.

The principal eigenvalue of (2.4) is guaranteed to be real, with a corresponding eigen-129 function ϕ that is real and sign definite (see Part I). This eigenfunction describes the 130 spatial structure of the concentration: according to (2.3) and the relation $q = \nabla_{\boldsymbol{\xi}} q$, the 131 structure of $C(\boldsymbol{x},t)$ at fixed t is locally proportional to $\phi(\boldsymbol{x},\boldsymbol{x}t)\exp(-\boldsymbol{q}\cdot\boldsymbol{x})$. Note that 132 the eigenvalue problem (2.4) also appears when the Floquet–Bloch theory of differential 133 equations with periodic coefficients is applied to (2.1) (see Bensoussan et al. 1989, §4.3.1; 134 Papanicolaou 1995, $\S3.6$), and in the problem of front propagation in the presence of an 135 FKPP chemical reaction (see Novikov & Ryzhik 2007; Xin 2009). 136

In Part I, we examine scalar dispersion in cellular flows by solving (2.4) numerically 137 for fixed Pe for a range of values q and then deducing $g(\boldsymbol{\xi})$ by Legendre transform. 138 We also provide an asymptotic approximation to f(q) in the limit Pe $\rightarrow 0$. Here we 139 obtain a detailed description in the opposite limit $Pe \rightarrow \infty$. This limit has received 140 a great deal of attention, most of which has been devoted to the determination of an 141 effective diffusivity k (Childress 1979; Shraiman 1987; Rosenbluth et al. 1987; Soward 142 1987; Fannjiang & Papanicolaou 1994; Koralov 2004; Novikov et al. 2005; Gorb et al. 143 2011). This characterises the dispersion for $\mathbf{x} = O(t^{1/2})$ by providing the (Gaussian) 144

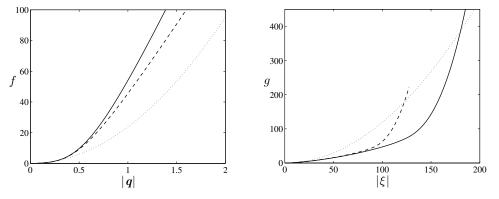


FIGURE 3. Eigenvalue $f(\mathbf{q})$ and rate function $g(\boldsymbol{\xi})$ for the cellular flow with Pe = 250 compared with the diffusive approximation (2.7). Left: $f(\mathbf{q})$ as a function of $|\mathbf{q}|$ for $\mathbf{q} = |\mathbf{q}|(1,1)/\sqrt{2}$ (solid line) and $\mathbf{q} = |\mathbf{q}|(1,0)$ (dashed line). Right: $g(\boldsymbol{\xi})$ as a function of $|\boldsymbol{\xi}|$ for $\boldsymbol{\xi} = |\boldsymbol{\xi}|(1,1)/\sqrt{2}$ (solid line) and $\boldsymbol{\xi} = |\boldsymbol{\xi}|(1,0)$ (dashed line). The diffusive approximation is shown by the dotted lines.

diffusive approximation $C(\boldsymbol{x},t) \approx \exp\left(-|\boldsymbol{x}|^2/(4\mathbf{k}t)\right)$ to the concentration. The key result in this area is the asymptotic approximation

$$\mathbf{k} \sim 2\nu \mathrm{Pe}^{1/2} \tag{2.5}$$

¹⁴⁷ (Childress 1979; Shraiman 1987; Rosenbluth et al. 1987; Soward 1987), where the constant

$$\nu = \left(\frac{2}{\pi}\right)^{1/2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^{1/2}} = 0.532740705\cdots$$
(2.6)

was determined by Soward (1987). This result is obtained by applying a boundary-layer analysis to the so-called cell problem which arises when computing an effective diffusivity using the method of homogenisation (e.g. Majda & Kramer 1999). Since the effective diffusivity can be deduced from the large-deviation functions f and g, specifically from their Taylor expansions

$$f(\boldsymbol{q}) \sim \mathbf{k} |\boldsymbol{q}|^2 \quad \text{and} \quad g(\boldsymbol{\xi}) \sim |\boldsymbol{\xi}|^2 / (4\mathbf{k})$$

$$(2.7)$$

for small q or $\boldsymbol{\xi}$ (see Part I), this result is recovered in our large-deviation treatment.

To illustrate the limitations of the diffusive approximation, we show in Figure 3 the 154 functions f(q) and $q(\boldsymbol{\xi})$ computed by numerically along straight lines in each of the q 155 and $\boldsymbol{\xi}$ planes for Pe = 250 (these curves correspond to cross sections of Figure 10 in Part 156 I). Both $f(\boldsymbol{q})$ and $q(\boldsymbol{\xi})$ differ strikingly from the parabolas of the diffusive approximation 157 with: a clear anisotropy indicating faster dispersion along the diagonal in the x plane 158 than along the axes; a q that is broader than parabolic in a intermediate range of x, 159 corresponding to concentrations exponentially larger than those predicted by diffusion; 160 and a sharp increase in g for large $\boldsymbol{\xi}$, corresponding to a localisation of the concentration. 161 The asymptotic theory presented in this paper explains these features. 162

Our derivation of the asymptotic form of $f(\mathbf{q})$ for $\text{Pe} \gg 1$ relies on a boundarylayer analysis of (2.4). Compared with that leading to the effective diffusivity (2.5), this derivation is complicated by the presence of the parameter \mathbf{q} . We identify two different regimes, which we denote as I and II characterised by $|\mathbf{q}| = O(\text{Pe}^{-1/4})$ and $|\mathbf{q}| = O(1)$, respectively. Regime I is suggested by the approximation (2.5), which implies that $f(\mathbf{q}) \propto |\mathbf{q}|^2 = O(\text{Pe}^{-1/2})$ for $|\mathbf{q}| \ll 1$. In this regime, the eigenvalue $f(\mathbf{q})$ is O(1)and is determined by matching a non-trivial solution in the interior of the flow cells with

a boundary-layer solution along the separatrices dividing the cells. The boundary-layer 170 problem for the whole of Regime I turns out to be identical to that arising in the ho-171 mogenisation approach and solved by Soward (1987). However, it is only in the limit 172 $\mathrm{Pe}^{-1/4}|\boldsymbol{q}| \to 0$ that the homogenisation solution, with ϕ constant in the cell interiors, 173 and the results (2.5)–(2.7) are recovered. In regime II, ϕ vanishes to leading order in the 174 cell interior, and the eigenvalue problem is entirely controlled by the behaviour in the 175 boundary layers. It turns out that $f(q) = O(\text{Pe}/\log \text{Pe})$ in this case. A third regime, ex-176 pected to arise for $|\mathbf{q}| = O(\text{Pe})$, is not considered here since it corresponds to exceedingly 177 small concentrations. It is commented upon the the conclusion of the paper. 178

We derive the solution f(q) in regimes I and II in sections §§ 3–4. The implications for 179 the rate function $q(\boldsymbol{\xi})$ are presented in § 5; this provides a more direct physical interpre-180 tation of the results since $q(\boldsymbol{\xi}) \sim t^{-1} \log C(\boldsymbol{x}, t)$ (see Part I, §2.2, for some remarks on 181 the qualitative links between f(q) and $q(\xi)$). The paper concludes with a brief discussion 182 in §6. Throughout the paper we use the following notational convention. In the period 183 $[0,2\pi] \times [0,2\pi]$ of the flow, two types of quarter cells of size $\pi \times \pi$ need to be distin-184 guished, depending on whether the flow circulates in the positive or negative direction 185 (see Figure 1). We denote by + the first type, and by - the second; when using \pm or \mp 186 for expressions with opposite signs in the different cells, the upper (lower) sign refers to 187 + (-) cells (so that $\psi = \pm 1$ at the centre of cells). 188

¹⁸⁹ **3. Regime I:** $|\boldsymbol{q}| = O(\text{Pe}^{-1/4})$

¹⁹⁰ To analyse this first regime, we introduce $\tilde{\boldsymbol{q}} = \operatorname{Pe}^{1/4} \boldsymbol{q}$ assumed to be O(1) and consider ¹⁹¹ separately the solution in the cell's interior and in a boundary layer around the separatri-¹⁹² ces. Note that the separatrices correspond to $\psi = 0$ and that, away from the stagnation ¹⁹³ points, ψ is a convenient coordinate with, for ψ small, ψ being proportional of the distance ¹⁹⁴ from the separatrix. As in the homogenisation problem (e.g. Childress 1979; Rosenbluth ¹⁹⁵ et al. 1987), the boundary-layer thickness scales like $\operatorname{Pe}^{-1/2}$; thus the cell interior is ¹⁹⁶ defined by $|\psi| \gg \operatorname{Pe}^{-1/2}$ while the boundary layer corresponds to $|\psi| = O(\operatorname{Pe}^{-1/2})$.

3.1. Interior problem

¹⁹⁸ Introducing the expansions

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 $\phi = \phi_0 + \operatorname{Pe}^{-1/4} \phi_1 + \operatorname{Pe}^{-1/2} \phi_2 + \cdots$ and $f = f_0 + \operatorname{Pe}^{-1/4} f_1 + \operatorname{Pe}^{-1/2} f_2 + \cdots$ (3.1)

¹⁹⁹ for the eigenfunction and eigenvalue into (2.4), we obtain

$$-\boldsymbol{u}\cdot\nabla\phi_0=0,\tag{3.2}$$

$$-\boldsymbol{u} \cdot \nabla \phi_j + \boldsymbol{u} \cdot \tilde{\boldsymbol{q}} \phi_{j-1} = 0, \quad j = 1, 2, 3, \tag{3.3}$$

$$\nabla^2 \phi_0 - \boldsymbol{u} \cdot \nabla \phi_4 + \boldsymbol{u} \cdot \tilde{\boldsymbol{q}} \phi_3 = f_0 \phi_0. \tag{3.4}$$

The solution to (3.2)–(3.3) is straightforward: it corresponds to the expansion in powers of Pe^{-1/4} of exp(Pe^{-1/4} $\tilde{\boldsymbol{q}} \cdot \boldsymbol{x})\Phi(\psi)$, where Φ is arbitrary. Thus, in each quarter-cell,

$$\sum_{j=0}^{3} \operatorname{Pe}^{-j/4} \phi_{j} = \operatorname{e}^{\operatorname{Pe}^{-1/4} \tilde{\boldsymbol{q}} \cdot \boldsymbol{x}} \sum_{j=0}^{3} \operatorname{Pe}^{-j/4} \Phi_{j}(\psi) + O(\operatorname{Pe}^{-1}),$$
(3.5)

where the functions Φ_i remain to be determined. In particular,

$$\phi_0 = \Phi_0(\psi). \tag{3.6}$$

²⁰³ Therefore, to leading order, the solution is constant along streamlines, in accordance

²⁰⁴ with familiar averaging results (cf. Rhines & Young 1983; Freidlin & Wentzell 1994). The

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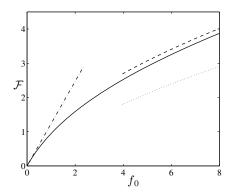


FIGURE 4. \mathcal{F} as defined by (3.10) as a function of f_0 . The numerical estimate of \mathcal{F} (solid line) is compared with asymptotic approximations for $f_0 \ll 1$ (dash-dotted line) and for $f_0 \gg 1$ (dashed line and dotted line, corresponding to two- and one-term asymptotic approximations).

higher-order terms in (3.5) are not periodic, but periodicity is restored through the rapid variation of ϕ across the boundary layer.

Eq. (3.4) can be solved for ϕ_4 provided that a solvability condition be satisfied. This solvability condition is obtained by integrating (3.4) along a streamline. Noting that the third term on the left-hand side can be written as $\boldsymbol{u} \cdot \tilde{\boldsymbol{q}} \phi_3 = \boldsymbol{u} \cdot \nabla(\cdots)$, where \cdots denotes a polynomial of degree 4 in $\tilde{\boldsymbol{q}} \cdot \boldsymbol{x}$ with ψ -dependent coefficients, this condition is found to be

$$\frac{\mathrm{d}}{\mathrm{d}\psi} \left(a(\psi) \frac{\mathrm{d}\Phi_0}{\mathrm{d}\psi} \right) = f_0 b(\psi) \Phi_0, \qquad (3.7)$$

212 where

$$a(\psi) = 8\left(E'(\psi) - \psi^2 K'(\psi)\right), \quad b(\psi) = 4K'(\psi),$$
(3.8)

and K' and E' are (complementary) complete elliptic integrals (e.g. DLMF 2010). Details of the derivation of (3.7)–(3.8) are given in Appendix A.1. Note that (3.7) can be recognised as an eigenvalue problem form of the diffusion equation obtained using averaging by Rhines & Young (1983), Freidlin & Wentzell (1994), Pauls (2006) and others.

As shown in Appendix A.1, the solution of (3.7) that is well behaved at the centres $\psi = \pm 1$ of the cell satisfies

$$\frac{\mathrm{d}\Phi_0}{\mathrm{d}\psi} = \pm \frac{f_0}{2} \Phi_0 \quad \text{at} \quad \psi = \mp 1. \tag{3.9}$$

Eq. (3.7) can be solved with this boundary condition and an arbitrary normalisation to find a linear relationship between Φ_0 and its derivative near the separatrices:

$$\frac{\mathrm{d}\Phi_0}{\mathrm{d}\psi} \sim \pm \mathcal{F}(f_0)\Phi_0 \quad \text{as} \quad \psi \to 0^{\mp}. \tag{3.10}$$

This defines the function $\mathcal{F}(f_0)$ (Dirichlet-to-Neumann map) which in practice needs to

be computed numerically. The boundary-layer analysis carried out in the next section determines the value of $\mathcal{F}(f_0)$ for a given q and hence gives the leading-order approximation $f_0(q)$ to the eigenvalue.

The form of $\mathcal{F}(f_0)$ obtained by solving (3.7)–(3.9) numerically is shown in Figure 4. Note that the fact that $\mathcal{F}(f_0)$ is positive implies that the solution decays away from the separatrices towards the centres of the cells. The asymptotic behaviour of \mathcal{F} for large

and small f_0 is useful. Computations detailed in Appendix A.1 give the following:

$$\mathcal{F}(f_0) \sim \frac{\pi^2 f_0}{8} \quad \text{as} \quad f_0 \to 0,$$
 (3.11)

$$\mathcal{F}(f_0) \sim \frac{\sqrt{2\lambda}}{4} \left(1 + \frac{\alpha}{\log \lambda} \right) \quad \text{as} \quad f_0 \to \infty.$$
 (3.12)

In (3.12), λ is a function of f_0 defined as the solution of

$$\lambda^2 = 4f_0 \log \lambda, \tag{3.13}$$

given explicitly in terms of a Lambert function in (A 11), and α is a constant given in (A 14). The crude approximation

$$\mathcal{F}(f_0) \sim \frac{(f_0 \log f_0)^{1/2}}{2} \text{ as } f_0 \to \infty$$
 (3.14)

is readily derived from (3.12) by neglecting the $O(\lambda/\log \lambda)$ term and using the leadingorder approximation $\lambda \sim (2f_0 \log f_0)^{1/2}$ to the solution of (3.13). This approximation is very poor, however, with a relative error decreasing to 0 only as $1/\log(\log f_0)$. The asymptotic approximations (3.11), (3.12) and (3.14) are compared with the numerical solution in Figure 4. This comparison validates the approximations and shows the importance of the logarithmic corrections to (3.14).

3.2. Boundary layer and matching

In the boundary layer surrounding the separatrices, rescaled variables need to be intro duced. Following Childress (1979), we let

$$\zeta = \mp \mathrm{Pe}^{1/2}\psi \quad \text{and} \quad \sigma = \int_0^l |\nabla \psi| \,\mathrm{d}l, \tag{3.15}$$

where l is the arclength along the separatrices. The sign in (3.15) is chosen such that $\zeta > 0$ in the interior of the quarter-cells. As detailed in Appendix A.2, $0 < \sigma < 8$ parameterises the boundary of each quarter-cell, with $\sigma = 0, 2, 4, 6$ at the corners (see Figure 1).

The eigenvalue f and eigenfunction ϕ are expanded as in (3.1), with the latter now regarded as a function of ζ and σ . Introducing into (2.4) gives

$$\partial_{\zeta\zeta}^2 \phi_0 - \partial_\sigma \phi_0 = 0, \qquad (3.16)$$

$$\partial_{\zeta\zeta}^2 \phi_1 - \partial_\sigma \phi_1 = -\frac{\boldsymbol{u} \cdot \tilde{\boldsymbol{q}}}{|\boldsymbol{u}|^2} \phi_0 \tag{3.17}$$

$$\partial_{\zeta\zeta}^2 \phi_2 - \partial_\sigma \phi_2 = -\frac{\boldsymbol{u} \cdot \tilde{\boldsymbol{q}}}{|\boldsymbol{u}|^2} \phi_1 \tag{3.18}$$

 $_{247}$ Eq. (3.16) has the constant solution

$$\phi_0 = \text{const.} = \Phi_0(0)$$

where $\Phi_0(0)$ is the limiting value of the leading-order interior solution on the separatrices. This indicates that the interior solution $\Phi_0(\psi)$ is the same in all quarter-cells. The problem posed by (3.17)–(3.18) is identical to the so-called Childress problem that arises in the computation of the effective diffusivity (Childress 1979). It was solved in closed form by Soward (1987) using a Wiener–Hopf technique and is discussed further in

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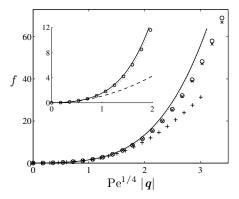


FIGURE 5. Eigenvalue $f(\mathbf{q})$ for the cellular flow as a function of $|\mathbf{q}|$ in regime I, with $\text{Pe} \gg 1$, $\text{Pe}^{1/4}\mathbf{q} = O(1)$. The asymptotic prediction (3.20) (solid line) is compared with numerical solutions of the eigenvalue problem for Pe = 5000 with $\mathbf{q} = |\mathbf{q}|(1,1)/\sqrt{2}$ (\circ) and $\mathbf{q} = (|\mathbf{q}|, 0)$ (\times), and for Pe = 500 with $\mathbf{q} = |\mathbf{q}|(1,1)/\sqrt{2}$ (+). The approximation of (3.20) valid for $\text{Pe}^{-1/4} \ll \mathbf{q} \ll 1$ that is deduced from (3.12) is also shown (dotted curve). The diffusive approximation (3.21), which holds for $\mathbf{q} \ll \text{Pe}^{-1/4}$, is shown in the inset magnifying the small- $|\mathbf{q}|$ region (dashed line).

²⁵³ Appendix A.2. The key result is that

$$\partial_{\zeta}\phi_1 \to 0 \quad \text{and} \quad \frac{\partial\phi_2}{\partial\zeta} \sim -\frac{\pi^2\nu}{4} |\tilde{q}|^2 \Phi_0(0) \quad \text{as} \quad \zeta \to \infty,$$
 (3.19)

where ν is as given in (2.6).

The leading-order approximation to the eigenvalue f(q) is now obtained by matching the interior and boundary solutions. Comparing (3.10) and (3.19) and taking the relation between ζ and ψ (3.15) into account leads to

$$\mathcal{F}(f_0) = \frac{\pi^2 \nu}{4} |\tilde{\boldsymbol{q}}|^2,$$

258 and hence

$$f(\boldsymbol{q}) \sim \mathcal{F}^{-1}\left(\frac{\pi^2 \nu}{4} |\tilde{\boldsymbol{q}}|^2\right),$$
 (3.20)

where \mathcal{F}^{-1} denotes the inverse of \mathcal{F} . This is the desired approximation to the eigenvalue 259 f(q) in regime I, with $\operatorname{Pe}^{1/4}q = O(1)$ as $\operatorname{Pe} \to \infty$. It is completely explicit apart from the 260 requirement for numerical solution of the ODE (3.7) in order to determine \mathcal{F} . It indicates, 261 in particular, that f(q) depends only on |q| in this regime, hence $g(\boldsymbol{\xi})$ depends only on 262 $|\boldsymbol{\xi}|$. Thus dispersion is isotropic not only in the diffusive regime but in the entire regime 263 I. As shown below, the anisotropy of the dispersion appears in regime II, for $q \gg \text{Pe}^{-1/4}$. 264 We have verified formula (3.20) by comparison with numerical estimates of f(q) ob-265 tained by solving a discretisation of the eigenvalue problem (2.4) on a 1000^2 grid (see 266 Part I for details). The results are summarised in Figure 5. The comparison between the 267 numerical estimates obtained for different values of Pe (500 and 5000), and for different 268 orientations of q (parallel to (1,1) and parallel to (1,0)) confirms the dependence of f269 on $\operatorname{Pe}^{1/4}|\boldsymbol{q}|$, the isotropy of the dispersion, and more generally the validity of (3.20). 270 Formula (3.20) can be simplified further using the asymptotic approximations (3.11)271

and (3.12) of \mathcal{F} for small and large argument. Using (3.11), (3.20) reduces to

$$f(\boldsymbol{q}) \sim 2\nu |\tilde{\boldsymbol{q}}|^2 = 2\nu \mathrm{Pe}^{1/2} |\boldsymbol{q}|^2 \quad \text{for} \quad \boldsymbol{q} \ll \mathrm{Pe}^{-1/4}$$
(3.21)

This can be recognised as the diffusive approximation: the effective diffusivity deduced from (2.7) recovers Soward's expression (2.5)–(2.6). On the other hand, (3.14) gives

$$f(\boldsymbol{q}) \sim \frac{\pi^4 \nu^2 \mathrm{Pe}|\boldsymbol{q}|^4}{16 \log \left(\mathrm{Pe}^{1/4} |\boldsymbol{q}| \right)} \quad \text{for } \mathrm{Pe}^{-1/4} \ll \boldsymbol{q} \ll 1.$$
(3.22)

The latter approximation is poor because of the neglect of logarithmic terms, but it is useful in suggesting that $f(\boldsymbol{q})$ is proportional to Pe/log Pe when \boldsymbol{q} is not small. The two asymptotic approximations are shown in Figure 5. For $\tilde{\boldsymbol{q}} \gg 1$, we used a better approximation than (3.22) obtained by inverting (3.12) numerically; this matches (3.20) accurately for $|\tilde{\boldsymbol{q}}| \gtrsim 1$.

280 4. Regime II: |q| = O(1)

In this regime, the eigenfunction vanishes to leading order in the cell interiors. The problem is then entirely controlled by the behaviour inside the boundary layers around the separatrices. In contrast with the situation for $|\mathbf{q}| = O(\text{Pe}^{-1/4})$, the dynamics in the corners of the cells – that is, near the stagnation points – plays a crucial role. The eigenvalue $f(\mathbf{q})$ scales roughly like Pe; it is therefore convenient to introduce

$$\mathbf{f}(\boldsymbol{q}) = \mathrm{Pe}^{-1} f(\boldsymbol{q}). \tag{4.1}$$

Note that f(q) is not O(1) but turns out to be $O(1/\log \text{Pe})$; however, to obtain a reasonably accurate approximation to the eigenvalue, it is important to capture logarithmic corrections: in what follows we therefore treat $1/\log \text{Pe}$ as an O(1) quantity and neglect only terms that are algebraic in Pe^{-1} .

290

4.1. Eigenvalue problem

Away from the corners, the leading-order boundary-layer equation obtained from (2.4) using the variables (3.15) is

$$\partial_{\zeta\zeta}^2 \phi - \partial_\sigma \phi + \frac{\boldsymbol{u} \cdot \boldsymbol{q}}{|\boldsymbol{u}|^2} \phi = \frac{\mathsf{f}}{|\boldsymbol{u}|^2} \phi, \qquad (4.2)$$

where u is evaluated on the separatrix. The solution can be written as

$$\phi = \mathrm{e}^{\boldsymbol{q} \cdot \boldsymbol{x} + \mathrm{f} H(\sigma)} \varphi, \tag{4.3}$$

²⁹⁴ where

$$H(\sigma) = \frac{1}{2} \log \frac{2-\sigma}{\sigma} \quad \text{for } 0 < \sigma < 2, \quad H(\sigma+2) = H(\sigma) \tag{4.4}$$

295 and the function φ satisfies the heat equation

$$\partial_{\zeta\zeta}^2 \varphi - \partial_\sigma \varphi = 0. \tag{4.5}$$

See Appendix B.1 for details. Note that since ϕ is periodic, φ is not, but there is a simple relation for the change in φ under a translation that represents a map from one '+' (or one '-') cell to another.

Eq. (4.2) breaks down near the corners $\sigma = 0, 2, 4, 6$, where u vanishes. There a different approximation to (2.4) needs to be considered; this provides a condition matching the form of ϕ downstream of the corners to its form upstream. The analysis of the corner region carried out in Appendix B.1 gives this condition as

$$\lim_{\sigma \to k^+} \varphi(\sigma, \zeta) = (16 \text{Pe})^{-f/2} \zeta^f \lim_{\sigma \to k^-} \varphi(\sigma, \zeta) \text{ for } k = 0, 2, 4, 6.$$

$$(4.6)$$

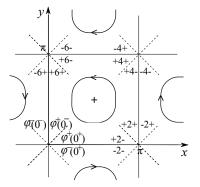


FIGURE 6. Set-up of the boundary-layer analysis in regime II. The function $\varphi^+(\sigma,\zeta)$ and $\varphi^-(\sigma,\zeta)$ denote φ respectively inside and outside of the separatrix around the central quarter-cell. The heat equation (4.5) relates the functions $\varphi^{\pm}(\sigma,\zeta)$ immediately upstream of each corner, that is, for $\sigma = 0^-$, 2^- , 4^- , 6^- , to the corresponding functions immediately downstream of each corner, that is, for $\sigma = 6^+$, 0^+ , 2^+ , 4^+ . These functions are indicated explicitly in the lower left corner $\sigma = 0$ (omitting the dependence on ζ), and symbolically in the other corners with, for instance, +2- denoting $\varphi^+(2^-, \zeta)$.

Eqs. (4.5)–(4.6), together with with the jump conditions between $[0, 2\pi]^2$ cells implied 303 by the 2π -periodicity of ϕ , form an eigenvalue problem with φ in each cell as eigenfunction 304 and f as eigenvalue. It is in fact sufficient to consider a single quarter-cell, say the + cell 305 centred centred at $(\pi/2, \pi/2)$: if $\varphi^+(\sigma, \zeta)$ and $\varphi^-(\sigma, \zeta)$ denote φ in the boundary layer 306 inside and outside this cell (so that φ^- straddles the four quarter-cells of type – adjacent 307 to the cell of type +, see Fig. 6), the periodicity of ϕ implies that the value of φ in all 308 other cells can be deduced from φ^{\pm} . Furthermore, since solving (4.5) between corners 309 provides a map between φ^{\pm} immediately downstream of each corner and φ^{\pm} immediately 310 upstream of the next corner, that is, between $\varphi^{\pm}(k^+,\zeta)$ and $\varphi^{\pm}(k+2^-,\zeta)$, the problem 311 can be formulated entirely in terms of $\varphi^{\pm}(k^+,\xi), k=0, 2, 4, 6$. Defining a vector 312

$$\varphi(\zeta) = (\varphi^+(0^+, \zeta), \varphi^-(0^+, \zeta), \varphi^+(2^+, \zeta), \varphi^-(2^+, \zeta), \cdots, \varphi^-(6^+, \zeta))^{\mathrm{T}}$$
(4.7)

 $_{313}$ grouping these 8 functions, we show in Appendix B.1 that the problem can be written $_{314}$ as

$$(16\text{Pe})^{f/2}\varphi = \mathcal{L}(q, f)\varphi.$$
(4.8)

Here $\mathcal{L}(\boldsymbol{q}, \mathsf{f})$ is an 8 × 8 matrix, given explicitly in (B 9), whose entries are simple linear integral operators.

Let $\mu(q, f)$ be the principal eigenvalue of $\mathcal{L}(q, f)$:

$$\mathcal{L}(\boldsymbol{q}, \boldsymbol{\mathsf{f}})\boldsymbol{\varphi} = \boldsymbol{\mu}(\boldsymbol{q}, \boldsymbol{\mathsf{f}})\boldsymbol{\varphi}. \tag{4.9}$$

Then f and hence f are found as a functions of Pe by solving

$$(16 \text{Pe})^{f/2} = \mu(q, f).$$
 (4.10)

This is the main result of this section. It gives the rate function f as Pe times the

solution f of the nonlinear equation (4.10). Since $f \to 0$ as $Pe \to \infty$, it is asymptotically

 $_{321}$ consistent to solve this equation approximately for small f, which yields the leading-order

322 approximation

$$f(\boldsymbol{q}) = \operatorname{Pef}(\boldsymbol{q}) \sim \frac{2\operatorname{Pe}}{\log \operatorname{Pe}} \log \mu(\boldsymbol{q}, 0).$$
(4.11)

However, as mentioned earlier, this approximation is poor since it makes a relative error

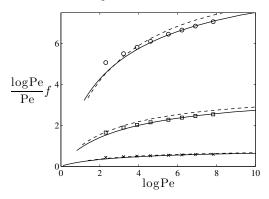


FIGURE 7. Scaled eigenvalue $f(\mathbf{q})$ as a function of Pe in regime II. The numerical solution of the eigenvalue problem (symbols) is compared with the asymptotic prediction (4.10) (solid lines) for $q_1 = q_2 = 0.5$ (×), 1 (□) and 2 (◦). As Pe $\rightarrow \infty$, log Pef/Pe slowly tends to the limiting values $2 \log \mu(\mathbf{q}, 0)$ given here by 0.85, 3.7 and 10.0. The heuristic formula (4.12) is indicated by the dashed lines.

of order $O(1/\log \text{Pe})$; it is therefore preferable to use (4.10) instead. A heuristic improvement on (4.11) retains the factor 16 inside the logarithm to read

$$f(\boldsymbol{q}) = \operatorname{Pef}(\boldsymbol{q}) \sim \frac{2\operatorname{Pe}}{\log(16\operatorname{Pe})} \log \mu(\boldsymbol{q}, 0).$$
(4.12)

In practice, we can obtain $\mu(q, f)$ numerically by computing the eigenvalues of a dis-326 cretised version of $\mathcal{L}(q, f)$ for a range of f, then deduce the corresponding values of Pe by 327 solving (4.10). Alternatively, if f is to be estimated for a fixed Pe, (4.10) can be solved for 328 f iteratively, starting with (4.11). Figure 7 demonstrates the accuracy of (4.10) by com-329 paring its prediction with the numerical solution of the full eigenvalue problem (2.4) for 330 f for values of Pe ranging from 10 to 2500 and for three different values of $q_1 = q_2$. The 331 figure indicates that (4.10) is useful for values of Pe as small as 100. It also confirms the 332 limited usefulness of the leading-order asymptotics (4.11): for $q_1 = q_2 = 2$, for instance, 333 the convergence of $\log \text{Pe} f/\text{Pe}$ to its limiting value $2\log \mu(q, 0) = 10.0$ is very slow so 334 that exceedingly large Pe are required for an acceptable approximation. The heuristic 335 formula (4.12), although of the same formal accuracy, provides a clear improvement. 336

To illustrate the validity of (4.10) over a broad range of q, we compare in Figure 8 337 this prediction with numerical solutions along the lines $q_2 = 0$ and $q_1 = q_2$ in the q-338 plane for Pe = 1000. The asymptotic prediction is virtually undistinguishable from the 339 full numerical solution for $|\mathbf{q}| \geq 0.5$. The figure confirms the anisotropy of dispersion in 340 regime II. A two-dimensional plot of f (see Figure 10 in Part I) indicates that the shape 341 of constant-f contours changes from circular for small values to straight segments given 342 by $|q_1| + |q_2| = \text{const.}$ for large values. The behaviour is confirmed explicitly in the next 343 subsection. 344

345

4.2. Asymptotic limits

The asymptotics of $f(\mathbf{q})$ for large and small $|\mathbf{q}|$ is of interest. For simplicity, we consider the limit $|\mathbf{q}| \ll 1$ in the approximation (4.11), that is, we neglect terms that are $O(1/\log \text{Pe})$. A calculation detailed in Appendix B.2 relates the eigenvalue problem for $|\mathbf{q}| \ll 1$ to that of the $|\mathbf{q}| = O(\text{Pe}^{-1/4})$ regime and yields

$$f(\boldsymbol{q}) \sim \frac{\pi^4 \nu^2 \operatorname{Pe}|\boldsymbol{q}|^4}{4 \log \operatorname{Pe}},\tag{4.13}$$

Dispersion in the large-deviation regime II

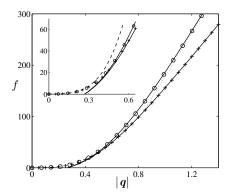


FIGURE 8. Eigenvalue $f(\mathbf{q})$ for the cellular flow for Pe = 1000 as a function of $|\mathbf{q}|$. The asymptotic prediction (4.10) (solid line) is compared with numerical solutions of the full eigenvalue problem (2.4) with $\mathbf{q} = |\mathbf{q}|(1,1)/\sqrt{2}$ (\circ) and $\mathbf{q} = (|\mathbf{q}|, 0)$ (+). The approximation valid for $q_1, q_2 \gg 1$ that is deduced from (4.15) is also shown (dotted line). The approximation (3.20) valid for $|\mathbf{q}| = O(\text{Pe}^{-1/4})$ is shown in the inset magnifying the small- $|\mathbf{q}|$ region (dashed line).

which matches the limiting form (3.22) of the $|\mathbf{q}| = O(\text{Pe}^{-1/4})$ regime. This shows that regimes I and II overlap in the region $\text{Pe}^{-1/4} \ll |\mathbf{q}| \ll 1$ where $f(\mathbf{q})$ is quartic in $|\mathbf{q}|$.

For $|\mathbf{q}| \gg 1$, the eigenvalue problem (4.8) can be greatly simplified by retaining only the dominant elements of the matrix $\mathcal{L}(\mathbf{q}, \mathsf{f})$. Specifically, assuming that both $|q_1|$ and $|q_2|$ are large, the eigenvalue $\mu(\mathbf{q}, \mathsf{f})$ can be approximated as

$$\mu(\mathbf{q}, \mathbf{f}) \sim e^{\pi(|q_1| + |q_2|)/2} \hat{\mu}(\mathbf{f}), \tag{4.14}$$

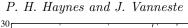
where $\hat{\mu}(f)$ is the eigenvalue of the (*q*-independent) scalar operator $\zeta^{f}\mathcal{H}_{-}$, with \mathcal{H}_{-} defined in (B8). This leads to the approximation

$$f \sim \frac{\text{Pe}}{\log(16\text{Pe})} \left[\pi(|q_1| + |q_2|) + 2\log\hat{\mu}(f/\text{Pe}) \right].$$
 (4.15)

The first term in the square brackets is asymptotically dominant, but for practical values of Pe the second term needs to be taken into account (so that (4.15) needs to be solved iteratively for f). Interestingly, (4.15) can be related to the large-deviation statistics of random walks: a random walk on a two-dimensional lattice, with steps of size $\pm a$ taken with probability 1/2 at time intervals τ , is characterised by a large-deviation function

$$f(\boldsymbol{q}) = \frac{1}{\tau} \log \left(\cosh(q_1 a) \cosh(q_2 a) \right) \sim \frac{a}{\tau} (|q_1| + |q_2|) \quad \text{as} \quad |\boldsymbol{q}| \to \infty,$$

assuming independent walks in the x- and y-directions. Comparison with (4.15) shows 362 that for large Pe and large |q|, the dispersion by a cellular flow is equivalent to a random 363 walk on the lattice of the hyperbolic stagnation points, with time intervals $\tau \propto \log Pe/Pe$ 364 between the steps. This scaling is natural: Pe/logPe is the time scale for both approach-365 ing the hyperbolic stagnation points along their stable manifold and for escaping from 366 their neighbourhood along their unstable manifold (as consideration of the simple one-367 dimensional problems $dX = \mp \operatorname{Pe} \sin X \, dt + \sqrt{2} \, dW$ readily confirms.) The physical inter-368 pretation is straightforward: since large values of q correspond to large distances, f(q)369 then describes the dispersion statistics of rare particles which travel anomalously fast 370 away from their point of release. As Figure 2 suggests, such particles move rapidly by 371 remaining near the separatrices. The $O(\log \text{Pe}/\text{Pe})$ time they take to pass through the 372 regions surrounding stagnation points is asymptotically larger than the O(1/Pe) time 373



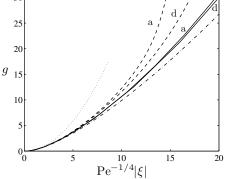


FIGURE 9. Rate function $g(\boldsymbol{\xi})$ as a function of $\operatorname{Pe}^{-1/4}|\boldsymbol{\xi}|$ for $\operatorname{Pe} = 100$ (dashed lines) and $\operatorname{Pe} = 500$ (solid lines). Numerical estimates for $\boldsymbol{x} = |\boldsymbol{\xi}|(1,1)/\sqrt{2}$ (labelled by 'd' for diagonal) and for $\boldsymbol{\xi} = |\boldsymbol{\xi}|(1,0)$ (labelled by 'a' for axis) are compared with the asymptotic approximation (5.1) (dash-dotted line). The quadratic diffusive approximation (2.7) is also shown (dotted line).

spent along the separatrix between these passages. From the current stagnation point a particle may move along the unstable manifold to one of the two connected stagnation points. As a result, the dynamics is approximated by that of a random walk with instantaneous jumps between neighbouring stagnation points.

Figure 8 confirms the asymptotics (4.15) by comparing its prediction with a numerical 378 estimate for f(q) for Pe = 1000 and $q_1 = q_2$. The asymptotics is accurate for $q_1 = q_2 \gtrsim 1$, 379 not surprisingly perhaps since the large parameter is in fact $\min(\exp(\pi q_1), \exp(\pi q_2))$ (see 380 B.2). The asymptotics does not apply in the case $q_2 = 0$ also shown in the Figure and 381 more generally if either q_1 or q_2 is O(1); it is not difficult to obtain a simplified formula 382 for this case, but this requires the eigenvalue of an operator more complicated than $\zeta^{\dagger}\mathcal{H}_{-}$. 383 Figure 8 also illustrates the switchover between regime I and regime II that occurs in the 384 range $\operatorname{Pe}^{-1/4} \ll |\boldsymbol{q}| \ll 1$ where the approximations (3.20) and (4.10) are both valid and 385 overlap. 386

We emphasise that the validity of the approximation given here for $|q| \gg 1$ is limited: 387 for $|\mathbf{q}| = O(\text{Pe})$ or larger, terms of (2.4) that are neglected in our boundary-layer treat-388 ment, most obviously the term $|\mathbf{q}|^2 \phi$, become important. For $|\mathbf{q}| \gg 1$ this term dominates 389 so that $f(q) \sim |q|^2$, corresponding to a purely diffusive behaviour. Physically, this de-390 scribes the statistics of particles that are so far from their release point that advection, 391 with the limits imposed by the finite velocity, can no longer be the dominant mechanism 392 of dispersion. The transition between our regime II and this diffusion-dominated regime 393 can be expected to take place in a third regime such that $|\mathbf{q}| = O(\text{Pe})$ (up to logarithmic 394 corrections); we leave the study of this regime for future work. 395

5. Rate function

In this section, we express the asymptotic results of §§ 3–4 in terms of the rate function $g(\boldsymbol{\xi})$. This is straightforward, since it only involves taking the Legendre transform of the (semi-)analytic formulas obtained for $f(\boldsymbol{q})$; it is useful however because, according to (2.3), the rate function directly provides the form of the scalar concentration.

The two regimes I and II identified for $f(\mathbf{q})$ naturally have counterparts for $g(\boldsymbol{\xi})$. Regime I, which assumes $\mathbf{q} = O(\text{Pe}^{-1/4})$, is valid for $|\mathbf{q}| \ll 1$ and yields $f(\mathbf{q}) = O(1)$, is readily seen to correspond to $\boldsymbol{\xi} = O(\text{Pe}^{1/4})$ and hold for $|\boldsymbol{\xi}| \ll \text{Pe}/\log \text{Pe}$. The Legendre Dispersion in the large-deviation regime II

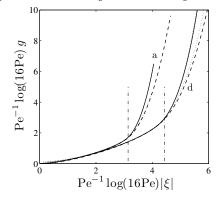


FIGURE 10. Rate function $g(\boldsymbol{\xi})$ in the scaling of Regime II for for Pe = 100 (dashed lines) and Pe = 500 (solid lines). Numerical estimates for $\boldsymbol{x} = |\boldsymbol{\xi}|(1,1)/\sqrt{2}$ (labelled by 'd' for diagonal) and for $\boldsymbol{\xi} = |\boldsymbol{\xi}|(1,0)$ (labelled by 'a' for axis) are compared with the asymptotic approximation derived from (4.10) (dotted line, shown for $\boldsymbol{\xi}$ along the diagonal only). The dash-dotted vertical segments indicate the vertical asymptotes (5.3) predicted for $\text{Pe} \to \infty$.

 $_{404}$ transform of (3.20) corresponds to a rate function of the form

$$g(\boldsymbol{\xi}) \sim \mathcal{G}(\operatorname{Pe}^{-1/4}|\boldsymbol{\xi}|),$$
(5.1)

where the function \mathcal{G} , essentially the Legendre transform of \mathcal{F}^{-1} in (3.20) can be com-405 puted numerically. This prediction is verified in Figure 9 which shows $g(\boldsymbol{\xi})$ as a function 406 of the scaled variable $Pe^{-1/4}|\boldsymbol{\xi}|$ for Pe = 100 and 500 and two different orientations of 407 $\boldsymbol{\xi}$. As predicted, for $\operatorname{Pe}^{-1/4}|\boldsymbol{\xi}|$ not too large, the curves obtained by numerical solution 408 of the eigenvalue problem collapse and match that obtained from the asymptotic solu-409 tion. The diffusive approximation, with the quadratic q given in (2.7), is also shown. The 410 physical implications of the results for regime I derived from f(q) can be reiterated based 411 on the form of $q(\boldsymbol{\xi})$: dispersion is isotropic in regime I, and the diffusive approximation 412 considerably underestimates the dispersion, with $g(\boldsymbol{\xi})$ much flatter than quadratic away 413 from $|\boldsymbol{\xi}| \ll \mathrm{Pe}^{1/4}$, corresponding to exponentially higher concentrations than predicted 414 by the effective diffusivity. The spatial distribution of the passive-scalar concentration, 415 governed by the eigenfunction $\phi(\boldsymbol{x},\boldsymbol{\xi})$, is shown in Part I: in regime I, the concentration 416 has a non-trivial distribution in the cell interior with similar values in the boundary layer 417 around the separatrices. As $\boldsymbol{\xi}$ increases from 0, the interior concentration changes from 418 near uniform to almost zero, with the boundary layer containing essentially all the scalar 419 for $|\boldsymbol{\xi}| \gg \mathrm{Pe}^{1/4}$. 420

The scaling of $g(\boldsymbol{\xi})$ is regime II can be obtained from (4.12) with the caveat that neglect of some logarithmic terms limits the accuracy of the expression derived in this manner. The orders of magnitude $\boldsymbol{q} = O(1)$ and $f(\boldsymbol{q}) = O(\text{Pe}/\log\text{Pe})$ associated with regime II correspond to $\boldsymbol{\xi} = O(\text{Pe}/\log\text{Pe})$ and $g(\boldsymbol{\xi}) = O(\text{Pe}/\log\text{Pe})$. More specifically, it follows from (4.12) that the rate function has the form

$$g(\boldsymbol{\xi}) \sim \frac{\mathrm{Pe}}{\mathrm{log}(16\mathrm{Pe})} \tilde{\mathcal{G}}\left(\frac{\mathrm{log}(16\mathrm{Pe})}{\mathrm{Pe}}\boldsymbol{\xi}\right)$$
 (5.2)

for some function $\tilde{\mathcal{G}}$ deduced from $\mu(\boldsymbol{q}, 0)$. As (4.12) itself this is an asymptotically inconsistent expression, taking into account the factor 16 inside the logarithms while neglecting other terms of the same, $O(1/\log \text{Pe})$ order. (The rate function deduced from f obtained by solving (4.10) gives a better approximation, but it is transcendental in

the Péclet number.) Figure 10 illustrates the behaviour of g in regime II by showing the same numerical results as in Figure 9 but with g and $\boldsymbol{\xi}$ scaled according to (5.2). For Pe⁻¹log(16Pe) \leq 1, the pairs of curves corresponding to the same $\boldsymbol{\xi}$ but different Péclet numbers (100 and 500) collapse, consistent with (5.2). For somewhat larger $\boldsymbol{\xi}$, the logarithmic corrections neglected matter, and the approximation derived from (4.10) then provides the required approximation.

The most striking feature in the behaviour of $g(\boldsymbol{\xi})$ is the abrupt increase once $|\boldsymbol{\xi}|$ exceeds a certain threshold. This implies that the concentration of a passive scalar drops suddenly for distances larger than t times this threshold and, in practice, means that scalar is effectively localised to a finite support. This feature is captured by expression (4.15) which provides an approximation of $f(\boldsymbol{q})$ for large \boldsymbol{q} . Ignoring the correction term involving $\hat{\mu}(f/\text{Pe})$, the Legendre transform of (4.15) implies that

$$g(\boldsymbol{\xi}) \to \infty \quad \text{as} \quad \max\left(|\xi_1|, |\xi_2|\right) \to \xi_* = \frac{\pi \text{Pe}}{\log(16\text{Pe})}.$$
 (5.3)

This provides an approximation for the size (and square shape) of this finite support for 442 $Pe \rightarrow \infty$. The finite support is entirely as expected for random walks with finite jumps 443 separated by finite time intervals (e.g. Keller 2004) which, as we have argued above, 444 applies in the large Pe regime. For large-but-finite Pe, the increase of $q(\boldsymbol{\xi})$ with $|\boldsymbol{\xi}|$ is in 445 fact smooth; it is encoded in $\hat{\mu}(f/\text{Pe})$ and for $|\xi_1|$ or $|\xi_2|$ substantially larger than ξ_* , 446 by the form of f(q) in the third regime q = O(Pe). However, the scalar concentrations 447 corresponding such values of $\boldsymbol{\xi}$ (that is, such distances to the scalar-release point) are 448 very small indeed. 449

450 6. Conclusion

The large-deviation approach developed in Part I and extended here makes it possible 451 to capture the tails in the distribution of a passive scalar released in the cellular flow 452 (1.1). It goes much further than the homogenisation approach classically applied to this 453 problem: while homogenisation describes only the Gaussian core of the scalar distribution 454 characterised by $|\mathbf{x}| = O(t^{1/2})$, the large-deviation approach gives the prediction of a 455 dependence in $\exp(-tq(\boldsymbol{x}/t))$ valid for much larger distances $|\boldsymbol{x}| = O(t)$. It furthermore 456 provides a method for determining the rate function g by solving a family of eigenvalue 457 problems. 458

The asymptotic analysis of these eigenvalue problems in the large-Péclet-number limit 459 reveals two district regimes in the dispersion. It is useful to summarise the predictions 460 in these regimes using dimensional variables. Regime I holds for moderately large dis-461 tances from the release point, specifically distances that satisfy $|\mathbf{x}| \ll Ut/\log \text{Pe}$. It is 462 characterised by an isotropic concentration that is broader than Gaussian and is con-463 trolled by the exchanges between the cell interiors across the separatrix regions. Regime 464 II holds for $(\kappa^3 U/a^3)^{1/4} t \ll |\mathbf{x}| = O(Ut/\log \text{Pe}) \ll Ut$, is anisotropic and characterised 465 by a sharp decrease of the concentration when $\max(|x|, |y|)$ approaches the specific value 466 $\pi Ut/\log(16 \text{Pe})$. Regime II describes the statistics of particles that remain near the sepa-467 ratrix at all times. The main factor limiting the concentration is then the passage through 468 the stagnation points; near the sharp concentration decrease, the evolution is analogous 469 to that of a random walk on the lattice formed by the stagnation points. For distances 470 larger still, the concentration is exceedingly small and controlled by a different physical 471 process in which molecular diffusion plays a key part; we do not analyse the corresponding 472 regime III in this paper. 473

⁴⁷⁴ While this paper is entirely devoted to dispersion of passive scalars, the results are also

relevant to problems involving reacting scalars. Specifically, the speed of propagation of 475 fronts in models such as the FKPP equation turns out to be controlled by the large-476 deviation rate function $q(\boldsymbol{\xi})$ for the corresponding passive-scalar problem (Gärtner & 477 Freidlin 1979; Freidlin 1985). Thus the asymptotic results of this paper can serve as a 478 basis for new predictions for the propagation speed of fronts in cellular flows as studied, 479 e.g., by Abel et al. (2002) and Novikov & Ryzhik (2007). These predictions are presented 480 in papers by Tzella & Vanneste (2014a, b); these also discuss regime III which turns out 481 to be important for large reaction rates. 482

We conclude by noting that the form of the large-deviation theory used in this paper is 483 an additive one, in the sense that it applies to SDEs with additive noise (and is therefore 484 very close to Cramér's original theory for the sum of random numbers). Its multiplicative 485 counterpart, exemplified by SDEs with multiplicative noise, is also relevant to the passive-486 scalar problem. It applies to the finite-time Lyapunov exponents which measure the rate 487 of stretching experienced by line elements in a flow: for sufficiently mixing flows, their 488 statistics obey a large-deviation principle and, remarkably, there is a significant part of 489 parameter space in which the corresponding rate function controls the decay rate of the 490 variance of passive scalars in such flows (e.g. Tsang et al. 2005; Haynes & Vanneste 2005). 491

Acknowledgments. The authors thank A. Tzella for useful discussions. JV acknowl edges support from grant EP/I028072/1 from the UK Engineering and Physical Sciences
 Research Council.

⁴⁹⁵ Appendix A. Derivation details for $|q| = O(\text{Pe}^{-1/4})$

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⁴⁹⁷ We obtain the solvability condition (3.7) by integrating (3.4) along streamlines. To do ⁴⁹⁸ this, we introduce the time-like coordinate *s* such that

A.1. Interior solution

$$\frac{\mathrm{d}}{\mathrm{d}s} = \boldsymbol{u} \cdot \nabla, \quad \text{i.e.} \quad \mathrm{d}s = \frac{\mathrm{d}x}{\sin x \cos y} = -\frac{\mathrm{d}y}{\cos x \sin y}, \tag{A1}$$

that is used in conjunction with the value of the streamfunction ψ . We first note that

$$\oint (\boldsymbol{u} \cdot \nabla \phi_4 + (\boldsymbol{u} \cdot \tilde{\boldsymbol{q}}) \phi_3) \, \mathrm{d}s = 0,$$

where the integration is along a streamline, can be deduced from (3.5), specifically that ϕ_3 is a sum of products of functions of $\tilde{q} \cdot x$ and functions of ψ , and that fact that $\oint \boldsymbol{u} \cdot \nabla f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{s} = 0$ for any function $f(\boldsymbol{x})$. Integrating (3.4) along a streamline then gives

$$\oint \nabla^2 \phi_0 \,\mathrm{d}s = f_0 \oint \phi_0 \,\mathrm{d}s. \tag{A2}$$

Now, following Rhines & Young (1983), we use the arclength $dl = |\nabla \psi| ds$ to compute

$$\oint \nabla^2 \phi_0 \, \mathrm{d}s = \frac{\mathrm{d}}{\mathrm{d}\psi} \iint \nabla^2 \phi_0 \, \mathrm{d}x \mathrm{d}y = \frac{\mathrm{d}}{\mathrm{d}\psi} \oint \nabla \phi_0 \cdot \mathrm{d}\boldsymbol{l} = \frac{\mathrm{d}}{\mathrm{d}\psi} \left(\oint |\nabla \psi| \, \mathrm{d}l \, \frac{\mathrm{d}\phi_0}{\mathrm{d}\psi} \right)$$

and reduce (A 2) to the form (3.7), where

$$a(\psi) = \oint |\nabla \psi| dl = \oint |\nabla \psi|^2 ds \quad \text{and} \quad b(\psi) = \oint \frac{dl}{|\nabla \psi|} = \oint ds \tag{A3}$$

₅₀₅ can be recognised respectively as the circulation and the orbiting time around streamlines.

The explicit expressions (3.8) for $a(\psi)$ and $b(\psi)$ are obtained as follows. To compute

 $b(\psi)$, we eliminate y from (A 1) using the constancy of $\psi = -\sin x \sin y$ and compute 507

$$b(\psi) = 2 \int_{\sin^{-1}\psi}^{\pi - \sin^{-1}\psi} \frac{\mathrm{d}x}{\sqrt{\sin^2 x - \psi^2}} = 4K'(\psi),$$

where $K'(\psi) = K(\sqrt{1-\psi^2})$ is a complete elliptic integral of the first kind (DLMF 2010), 508 and we have temporarily assumed that $0 \le \psi \le 1$. For $a(\psi)$, we observe that 509

$$a(\psi) = \iint \nabla^2 \psi \, \mathrm{d}x \mathrm{d}y = -2 \iint \psi \, \mathrm{d}\psi \mathrm{d}s = -2 \int \psi \mathrm{d}\psi \oint \mathrm{d}s = -2 \int \psi b(\psi) \, \mathrm{d}\psi,$$

and hence that 510

$$\frac{\mathrm{d}a}{\mathrm{d}\psi} = -2\psi b(\psi).$$

This equation can be integrated: using formula (19.4.2) in DLMF (2010) we obtain 511

$$a(\psi) = 8\left(E'(\psi) - \psi^2 K'(\psi)\right),\,$$

where $E'(\psi) = E(\sqrt{1-\psi^2})$ is a complete elliptic integral of the second kind. 512 The following properties of $a(\psi)$ and $b(\psi)$ are useful: 513

$$a(0) = 8, \qquad b(\psi) \sim 4\log(4/|\psi|) \text{ as } \psi \to 0,$$
 (A 4)

$$a(\psi) \sim 4\pi (1 \pm \psi) \text{ as } \psi \to \mp 1, \qquad b(\mp 1) = 2\pi.$$
 (A 5)

In particular, using (A5), a Frobenius expansion shows that solutions of (3.7) bounded 514 at $\psi = \mp 1$ have the form 515

$$\Phi_0 = C(1 + f_0(1 \pm \psi)/2 + O\left((1 \pm \psi)^2\right)),$$

where C in arbitrary constant (the other solutions have a logarithmic singularity). This 516 leads to the boundary condition (3.9). 517

We now consider the solution of (3.7) in the limits $f_0 \to 0$ and $f_0 \to \infty$ and derive the 518 asymptotic expressions (3.11)–(3.12) for $\mathcal{F}(f_0)$. For $f_0 \to 0$, $\Phi_0 = 1 + O(f_0)$; introducing 519 this in the right-hand side of (3.7), integrating and imposing boundedness gives 520

$$\frac{\mathrm{d}\Phi_0}{\mathrm{d}\psi} \sim \frac{f_0}{a(\psi)} \int_{\pm 1}^{\psi} b(\psi') \,\mathrm{d}\psi'$$

and hence 521

$$\mathcal{F}(f_0) \sim \frac{f_0}{a(0)} \int_0^1 b(\psi) \,\mathrm{d}\psi = \frac{\pi^2 f_0}{8}.$$

For $f_0 \to \infty$, it is convenient to introduce 522

$$r(\psi) = \frac{a(\psi)}{\Phi_0(\psi)} \frac{\mathrm{d}\Phi_0}{\mathrm{d}\psi} \tag{A6}$$

which satisfies the Riccati equation 523

$$\frac{\mathrm{d}r}{\mathrm{d}\psi} = f_0 b(\psi) - \frac{r^2}{a(\psi)}.\tag{A7}$$

The solutions of interest decay with $|\psi|$ and are approximated by 524

$$r = \pm \left(f_0 a(\psi) b(\psi) \right)^{1/2}$$

away from $\psi = 0$. (A boundary layer of $O(f_0^{-1})$ width appears around the centres $\psi = \pm 1$ 525

so that the boundary condition (3.9) can be satisfied.) 526

⁵²⁷ Near $\psi = 0$, (A 7) is approximated as

$$\frac{\mathrm{d}r}{\mathrm{d}\psi} = 4f_0 \log(4/|\psi|) - \frac{1}{8}r^2 + O(f_0\psi^2).$$
(A8)

⁵²⁸ using (A 4). A dominant-balance argument suggests to introduce

$$\Psi = \lambda \psi$$
 and $R = r/\lambda$, (A.9)

529 where λ satisfies

$$\lambda^2 = 4f_0 \log \lambda \tag{A 10}$$

530 Note that this equation has the closed-form solution

$$\lambda = \exp\left(-\frac{W_{\rm m}(-1/(2f_0))}{2}\right) \tag{A 11}$$

in terms of the Lambert function $W_{\rm m}$ (e.g. DLMF 2010), and the approximate solution

$$\lambda \sim (2f_0 \log f_0)^{1/2}$$
 as $f_0 \to \infty$.

532 Introducing (A 9) transforms (A 8) into

$$\frac{\mathrm{d}R}{\mathrm{d}\Psi} = 1 - \frac{R^2}{8} + \frac{\log(4/|\Psi|)}{\log\lambda} + O(1/(\lambda\log\lambda)),\tag{A 12}$$

where we assume $\Psi = O(1)$. We solve this equation perturbatively: the expansion

$$R = \pm 2\sqrt{2} + \frac{R_1}{\log \lambda} + O\left(1/(\lambda \log \lambda)\right), \qquad (A\,13)$$

where $R_1(\psi)$ remains to be determined, satisfies (A 12) to leading order. At the next order, we find

$$\frac{\mathrm{d}R_1}{\mathrm{d}\Psi} = \pm \frac{\sqrt{2}}{2}R_1 + \log \frac{4}{|\Psi|}$$

536 The solution that is bounded as $|\Psi| \to \infty$ takes the form

$$R_1 = \mp \sqrt{2} \log(|\Psi|/4) \mp \sqrt{2} e^{\sqrt{2}|\Psi|/2} \operatorname{Ei}(\sqrt{2}|\Psi|/2),$$

where Ei is the exponential integral (e.g. DLMF 2010). Evaluating at $\Psi = 0$ gives

$$R_1(0) = \pm \frac{\sqrt{2}}{2} (3 \log 2 + 2\gamma),$$

where γ is Euler's constant. After introducing this result into (A 13), we find from (A 9), (A 6) and (A 4) that

$$\mathcal{F}(f_0) \sim \frac{\sqrt{2\lambda}}{4} \left(1 + \frac{\alpha}{\log \lambda} \right), \quad \text{where} \quad \alpha = \frac{3\log 2 + 2\gamma}{4} = 0.8084682178\cdots.$$
 (A 14)

540

A.2. Boundary-layer solution

The boundary layer equations (3.17)–(3.18) are essentially identical to those to be solved to compute the effective diffusivity using a homogenisation approach. Thus the solution follows closely Childress (1979) and Soward (1987) and is detailed here for completeness (see also Childress & Soward 1989).

Since the solution is identical in the quarter-cells with the same sense of flow rotation, we concentrate on the + quarter-cell $[0, \pi] \times [0, \pi]$ and on the - cell $[0, \pi] \times [\pi, 2\pi]$. We

note that 547

$$0 < \sigma = 1 - \cos x < 2$$
 for $y = 0$, $2 < \sigma = 3 - \cos y < 4$ for $x = \pi$,
 $4 < \sigma = 5 + \cos x < 6$ for $y = \pi$, $6 < \sigma = 7 + \cos y < 8$ for $x = 0$.

in the + quarter-cell, while 548

$$\begin{array}{l} 0 < \sigma = 1 - \cos x < 2 \ \ \text{for} \ \ y = 2\pi, \ 2 < \sigma = 3 - \cos y < 4 \ \text{for} \ \ x = \pi, \\ 4 < \sigma = 5 + \cos x < 6 \ \ \text{for} \ \ y = \pi, \ 6 < \sigma = 7 + \cos y < 8 \ \text{for} \ \ x = 0. \end{array}$$

in the - quarter-cell. Eqs. (3.17)–(3.18) are solved in these two quarter-cells. This leads 549 to solutions $\phi_k^{\pm}(\sigma,\zeta)$, k=1,2, that need to be matched across the separatrice $\zeta=0$. 550 Using periodicity, the matching conditions are found to be 551

$$\phi_k^+(\sigma,0) = \phi_k^-(\sigma,0) \quad \text{and} \quad \partial_\zeta \phi_k^+(\sigma,0) = -\partial_\zeta \phi_k^-(\sigma,0) \quad \text{for} \quad 0 < \sigma < 2, \ 4 < \sigma < 6, \\ \phi_k^+(\sigma,0) = \phi_k^-(\sigma+4,0) \quad \text{and} \quad \partial_\zeta \phi_k^+(\sigma,0) = -\partial_\zeta \phi_k^-(\sigma+4,0) \quad \text{for} \quad 2 < \sigma < 4, \ 6 < \sigma < 8, \\ \phi_k^+(\sigma,0) = \phi_k^-(\sigma+4,0) \quad \text{and} \quad \partial_\zeta \phi_k^+(\sigma,0) = -\partial_\zeta \phi_k^-(\sigma+4,0) \quad \text{for} \quad 2 < \sigma < 4, \ 6 < \sigma < 8, \\ \phi_k^+(\sigma,0) = \phi_k^-(\sigma+4,0) \quad \text{and} \quad \partial_\zeta \phi_k^+(\sigma,0) = -\partial_\zeta \phi_k^-(\sigma+4,0) \quad \text{for} \quad 2 < \sigma < 4, \ 6 < \sigma < 8, \\ \phi_k^+(\sigma,0) = \phi_k^-(\sigma+4,0) \quad \text{and} \quad \partial_\zeta \phi_k^+(\sigma,0) = -\partial_\zeta \phi_k^-(\sigma+4,0) \quad \text{for} \quad 2 < \sigma < 4, \ 6 < \sigma < 8, \\ \phi_k^+(\sigma,0) = \phi_k^-(\sigma+4,0) \quad \text{and} \quad \partial_\zeta \phi_k^+(\sigma,0) = -\partial_\zeta \phi_k^-(\sigma+4,0) \quad \text{for} \quad 2 < \sigma < 4, \ 6 < \sigma < 8, \\ \phi_k^+(\sigma,0) = \phi_k^-(\sigma+4,0) \quad \text{and} \quad \partial_\zeta \phi_k^+(\sigma,0) = -\partial_\zeta \phi_k^-(\sigma+4,0) \quad \text{for} \quad 2 < \sigma < 4, \ 6 < \sigma < 8, \\ \phi_k^+(\sigma,0) = \phi_k^-(\sigma+4,0) \quad \text{for} \quad 2 < \phi_k^-(\phi+4,0) \quad \text{for} \quad 2 < \phi_k^-(\phi+4,0)$$

552

with the ϕ_k^{\pm} periodic with period 8 (see Fig. 1). Using that $\phi_0 = \Phi_0(0)$ is a constant, (3.17) is written explicitly as 553

$$\partial_{\zeta\zeta}^2 \phi_1^{\pm} - \partial_{\sigma} \phi_1^{\pm} = -\tilde{q}_1 F(\sigma) \mp \tilde{q}_2 F(\sigma - 2), \qquad (A \, 15)$$

where 554

$$F(\sigma) = \begin{cases} (2\sigma - \sigma^2)^{-1/2} & \text{for } 0 < \sigma < 2\\ 0 & \text{for } 2 < \sigma < 4 \end{cases} \quad \text{and} \quad F(\sigma + 4) = -F(\sigma).$$
(A 16)

For convenience, we have used the linearity of (3.17)–(3.18) to set $\phi_0 = \Phi_0(0) = 1$ 555 temporarily. 556

It follows from (A15)–(A16) that $\phi_1^{\pm}(\sigma + 4, \zeta) = -\phi_1^{\pm}(\sigma, \zeta)$ and so the matching 557 conditions become 558

$$\phi_1^+(\sigma, 0) = \phi_1^-(\sigma, 0) \text{ and } \partial_{\zeta} \phi_1^+(\sigma, 0) = -\partial_{\zeta} \phi_1^-(\sigma, 0) \text{ for } 0 < \sigma < 2, \ 4 < \sigma < 6 \text{(A 17)}$$

$$\phi_1^+(\sigma, 0) = -\phi_1^-(\sigma, 0) \text{ and } \partial_{\zeta} \phi_1^+(\sigma, 0) = \partial_{\zeta} \phi_1^-(\sigma, 0) \text{ for } 2 < \sigma < 4, \ 6 < \sigma < 8 \text{(A 18)}$$

Defining $G(\sigma)$ by 559

$$G'(\sigma) = F(\sigma)$$
 and $\int_0^8 G(\sigma) \, \mathrm{d}\sigma = 0,$ (A 19)

that is, 560

$$G(\sigma) = \begin{cases} \sin^{-1}(\sigma - 1) & \text{for } 0 < \sigma < 2, \\ \pi/2 & \text{for } 2 < \sigma < 4 \end{cases}, \quad G(\sigma + 4) = -G(\sigma),$$

the solution to (A 15)-(A 18) can be written as 561

$$\phi_1^{\pm}(\sigma,\zeta) = \tilde{q}_1 \left(G(\sigma) + \varrho(\sigma,\zeta) \right) \pm \tilde{q}_2 \left(G(\sigma-2) + \varrho(\sigma-2,\zeta) \right), \tag{A 20}$$

where $\rho(\sigma, \zeta)$ satisfies 562

$$\begin{aligned} \partial_{\zeta\zeta}^2 \varrho - \partial_{\sigma} \varrho &= 0, \ \partial_{\zeta} \varrho(\sigma, 0) = 0 \ \text{ for } \ 0 < \sigma < 2, \ 4 < \sigma < 6, \\ \varrho(\sigma, 0) &= -G(\sigma) \ \text{ for } \ 2 < \sigma < 4, \ 6 < \sigma < 8. \end{aligned}$$

Since $G(\sigma) = \pi/2$ for $2 < \sigma < 4$ and $G(\sigma) = -\pi/2$ for $6 < \sigma < 8$, 563

$$\varrho(\sigma,\zeta) = -\frac{\pi}{2}\theta(\sigma+2,\zeta), \qquad (A\,21)$$

⁵⁶⁴ where $\theta(\sigma, \zeta)$ satisfies

$$\begin{aligned} \partial_{\zeta\zeta}^2 \theta - \partial_{\sigma} \theta &= 0, \ \theta(\sigma, 0) = -1 \ \text{for} \ 0 < \sigma < 2, \\ \theta(\sigma, 0) &= 1 \ \text{for} \ 4 < \sigma < 6, \\ \partial_{\zeta} \theta(\sigma, 0) &= 0 \ \text{for} \ 2 < \sigma < 4, \ 6 < \sigma < 8 \end{aligned}$$

with $\theta \to 0$ as $\zeta \to \infty$. This is the problem solved in closed form by Soward (1987) using a Wiener-Hopf technique.

The solution (A 20) can now be introduced into Eq. (3.18) satisfied by ϕ_2 in order to obtain $\partial_{\zeta}\phi_2$ as $\zeta \to \infty$. We first rewrite (3.18) as

$$\partial_{\zeta\zeta}^2 \phi_2^{\pm} - \partial_{\sigma} \phi_2^{\pm} = -\left[\tilde{q}_1 F(\sigma) \pm \tilde{q}_2 F(\sigma-2)\right] \phi_1^{\pm},\tag{A 22}$$

and note that the leading-order behaviour of the solution as $\zeta \to \infty$ is controlled by the average in σ :

$$\phi_2^{\pm} \sim \bar{\phi}_2^{\pm} = \frac{1}{8} \int_0^8 \phi_2^{\pm} \,\mathrm{d}\sigma \ \ \mathrm{as} \ \ \zeta \to \infty.$$

⁵⁷¹ Introducing (A 20) into the average of (A 22) and using (A 19) and symmetries reduces ⁵⁷² this equation to

$$\partial_{\zeta\zeta}^2 \bar{\phi}_2^{\pm} = -\frac{|\tilde{\boldsymbol{q}}|^2}{4} \int_0^2 F(\sigma) \varrho(\sigma,\zeta) \,\mathrm{d}\sigma.$$

⁵⁷³ Integrating with respect to ζ then gives

$$\partial_{\zeta}\bar{\phi}_{2}^{\pm} = -\frac{|\tilde{\boldsymbol{q}}|^{2}}{4}\int_{0}^{2}F(\sigma)\int_{0}^{\infty}\varrho(\sigma,\zeta)\,\mathrm{d}\zeta\mathrm{d}\sigma = -\frac{\pi|\tilde{\boldsymbol{q}}|^{2}}{4}\int_{0}^{\infty}\varrho(0,\zeta)\,\mathrm{d}\zeta,$$

on using that $\partial_{\sigma} \int_{0}^{\infty} \varrho(\sigma, \zeta) d\zeta = -\partial_{\zeta} \varrho(\sigma, 0) = 0$ for $0 < \sigma < 2$. We finally obtain (3.19) using (A 21) above and formula (A.9) in Soward (1987), namely

$$\int_0^\infty \theta(2,\zeta) \,\mathrm{d}\zeta = -2\nu$$

where ν is defined by (2.6).

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⁵⁷⁷ Appendix B. Derivation details for |q| = O(1)

B.1. Boundary-layer solution

To solve (4.2), we note that $\partial_{\sigma}(\cdot) = \boldsymbol{u} \cdot \nabla(\cdot)/|\boldsymbol{u}|^2$, hence $\partial_{\sigma}\boldsymbol{x} = \boldsymbol{u}/|\boldsymbol{u}|^2$, and that $H(\sigma)$ defined in (4.4) satisfies

$$H(\sigma) = -\int_1^{\sigma} F^2(\sigma') \,\mathrm{d}\sigma' = -\int_1^{\sigma} \frac{\mathrm{d}\sigma'}{|\boldsymbol{u}(\sigma')|^2}$$

The undifferentiated terms in (4.2) can therefore be integrated explicitly to obtain (4.3)– (4.5). The periodicity of ϕ and the symmetry of the system imply the relationships

$$\varphi(x + k\pi, y + l\pi) = e^{-\pi(kq_1 + lq_2)}\varphi(x, y), \tag{B1}$$

for all integers k, l with k+l even. This makes it possible to deduce φ in all the boundary layers from its form φ^{\pm} on the interior and exterior sides of the boundary layer of the quarter-cell with centre at $(\pi/2, \pi/2)$.

We now obtain condition (4.6) governing the jump in φ at each corner. For definiteness, let us consider the corner at (0,0) of the + quarter-cell with centre at ($\pi/2, \pi/2$). Since - $xy \sim \psi = O(\text{Pe}^{-1/2})$ near this corner, suitable rescaled coordinates are $X = \text{Pe}^{1/4}x$; it terms of these, (2.4) reduces to

$$X\partial_X\phi - Y\partial_Y\phi + \mathsf{f}\phi = 0 \tag{B2}$$

⁵⁹⁰ to leading order in Pe. The solution is

$$\phi = X^{-f} \Phi(XY) \tag{B3}$$

for some function Φ that is found by matching with the solution (4.3) valid away from the corner. Upstream of the corner, this matching is made in the limit $Y \to \infty$ with $XY = \zeta$ fixed; noting that $Y = \text{Pe}^{1/4} y \sim \text{Pe}^{1/4} (-2\sigma)^{1/2}$ and $H(\sigma) \sim \log(-\sigma/2)/2$, we find

$$\Phi(\zeta) = (16 \text{Pe})^{-f/4} \zeta^f \lim_{\sigma \to 0^-} \varphi(\sigma, \zeta).$$
 (B4)

Note that we retain the factor ζ^{f} although it is asymptotically small since $\mathsf{f} \to 0$ as Pe $\to \infty$. This is because this leads to logarithmic corrections to f(q) which are not negligible for large-but-finite Pe.

⁵⁹⁸ Downstream of the corner the analogous matching corresponds to the limit $X \sim$ ⁵⁹⁹ $\operatorname{Pe}^{1/4}(2\sigma)^{1/2} \to \infty$ with $XY = \zeta$ fixed and leads to

$$\Phi(\zeta) = (16 \text{Pe})^{\mathsf{f}/4} \lim_{\sigma \to 0^+} \varphi(\sigma, \zeta) \tag{B5}$$

using that $H(\sigma) \sim \log(2/\sigma)/2$. Comparing (B 5) with (B 4) leads to the jump condition (4.6) at $\sigma = 0$. The same condition applies to all corners.

We are now in position to write down the eigenvalue problem determining f. The heat equation (4.5) makes it possible to relate the values of φ upstream of each corner to that downstream of the preceding corner. Specifically, integrating the heat equation for $0 < \sigma < 2$ gives

$$\varphi^{+}(2^{-},\zeta) = \mathcal{H}_{+}\varphi^{+}(0^{+},\zeta) + \mathcal{H}_{-}\varphi^{-}(0^{+},\zeta), \tag{B6}$$

$$\varphi^{-}(2^{-},\zeta) = \mathcal{H}_{-}\varphi^{+}(0^{+},\zeta) + \mathcal{H}_{+}\varphi^{-}(0^{+},\zeta), \tag{B7}$$

where \mathcal{H}_{\pm} are the linear operators giving the 'time'-2 flow of the heat equation and are defined by

$$\left(\mathcal{H}_{\pm}h\right)\left(\zeta\right) = \frac{1}{\sqrt{8\pi}} \int_0^\infty e^{-\left(\zeta \mp \zeta'\right)^2/8} h(\zeta') \,\mathrm{d}\zeta' \tag{B8}$$

for any function $h(\zeta)$.

Relations analogous to (B 6) can be written down for $\varphi^{\pm}(4^-, \zeta)$, $\varphi^{\pm}(6^-, \zeta)$ and $\varphi^{\pm}(8^-, \zeta) = \varphi^{\pm}(0^-, \zeta)$. The jump condition (4.6) can then be used to eliminate $\varphi^{\pm}(2k^-)$ in favour of $\varphi^{\pm}(2k^+)$. For φ^+ , this is straightforward: (4.6) gives

$$\varphi^+(0^+,\zeta) = (16\text{Pe})^{-f/2}\zeta^f\varphi^+(0^-,\zeta)$$

and similar relations at the other 3 corners. For φ^- , this is somewhat more complicated:

because φ^{-} is defined in 4 different quarter-cells, the upstream profiles are not immedi-

ately available. The periodicity conditions (B1) can however be used to express them in terms of $\varphi^{-}(2k^{-})$, see Figure 6. This leads to the jump conditions

$$\varphi^{-}(0^{+},\zeta) = (16\text{Pe})^{-f/2} e^{\pi(q_{1}+q_{2})} \zeta^{f} \varphi^{-}(4^{-},\zeta), \quad \varphi^{-}(2^{+},\zeta) = (16\text{Pe})^{-f/2} e^{\pi(q_{2}-q_{1})} \zeta^{f} \varphi^{-}(6^{-},\zeta),$$

$$\varphi^{-}(4^{+},\zeta) = (16\text{Pe})^{-f/2} e^{-\pi(q_{1}+q_{2})} \zeta^{f} \varphi^{-}(0^{-},\zeta), \quad \varphi^{-}(6^{+},\zeta) = (16\text{Pe})^{-f/2} e^{\pi(q_{2}-q_{1})} \zeta^{f} \varphi^{-}(2^{-},\zeta).$$

₆₁₆ Gathering these results, the eigenvalue problem can be written in the vector form (4.8)

617 where the linear operator \mathcal{L} is

618 with $a = e^{\pi q_1}$ and $b = e^{\pi q_2}$.

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B.2. Asymptotic limits

In the limit $|\mathbf{q} \ll 1$, the eigenvalue problem (4.9) or, equivalently, (4.2) can be solved by perturbation expansion in powers of $|\mathbf{q}|$. Since f decreases rapidly with $|\mathbf{q}|$ (like $|\mathbf{q}|^4$ as is verified below), the right-hand side of (4.2) and the jumps (4.6) are negligible. Expanding ϕ in powers of $|\mathbf{q}|$ then leads to the same sequence of equations (3.16)–(3.18) as considered in the $|\mathbf{q}| = O(\mathrm{Pe}^{-1/4})$ regime. The solution is the same: to leading-order ϕ is a constant, and the slope of the solution as $\zeta \to \infty$ is related to this constant according to (3.19). This implies that

$$\frac{\partial \boldsymbol{\varphi}}{\partial \zeta} \sim -\frac{\pi^2 \nu}{4} |\boldsymbol{q}|^2 \boldsymbol{\varphi} \quad \text{as} \quad \zeta \to \infty.$$
 (B 10)

⁶²⁷ This perturbative solution breaks down for large ζ , however, since the constant leading-⁶²⁸ order ϕ is inconsistent with the decay requirement for φ . For large ζ , the eigenfunction φ ⁶²⁹ takes an exponential form:

 $\varphi \propto \exp(-\lambda \zeta)$ as $\zeta \to \infty$

for some λ . Comparing with (B 10) gives

$$\lambda = \frac{\pi^2 \nu}{4} |\boldsymbol{q}|^2. \tag{B11}$$

It can be verified that the decay rate λ is related to the eigenvalue $\mu(q, 0)$ by

$$\mu(\boldsymbol{q},0) = \mathrm{e}^{2\lambda^2}.\tag{B12}$$

 $_{632}$ Combining (4.11), (B11) and (B12) yields the approximation (4.13).

For $|q_1|$, $|q_2| \gg 1$, the eigenvalue problem (4.9) simplifies dramatically. For definiteness, we assume $q_1, q_2 > 0$. In this case, $a^{-1}b^{-1} \ll 1 \ll ab$ in (B9). This implies that φ_2 , the second component of φ , is its largest component, and that $\varphi_4 \ll \varphi_2 \ll \varphi_3$. Taking this into account reduces (4.9) to

$$\mu \left(\begin{array}{c} \varphi_2\\ \varphi_3 \end{array}\right) = \zeta^{\mathsf{f}} \left(\begin{array}{c} 0 & ab\mathcal{H}_-\\ \mathcal{H}_- & 0 \end{array}\right) \left(\begin{array}{c} \varphi_2\\ \varphi_3 \end{array}\right),$$

637 and hence to

$$\mu^2 \varphi_2 = ab\zeta^{2\mathsf{f}} \mathcal{H}_-^2 \varphi_2.$$

Therefore, $\mu(\mathbf{q}, \mathbf{f}) = (ab)^{1/2}\hat{\mu}(\mathbf{f})$, where $\hat{\mu}(\mathbf{f})$ is the eigenvalue of $\zeta^{\mathbf{f}}\mathcal{H}_{-}$ and (4.14) follows.

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