Asymptotics for Strong Localized Perturbations: Theory and Applications

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(*23 November 2010*)

1 Introduction

The method of matched asymptotic expansions is a powerful systematic analytical method for asymptotically calculating solutions to singularly perturbed PDE problems. It has been successfully used in a wide variety of applications (cf. [**35**], [**42**]).

In these workshop notes we consider various classes of perturbation problems with localized imperfections in multi-dimensional domains. A perturbation of large magnitude but small extent will be called a strong localized perturbation. It may be contrasted with a weak perturbation, which is of small magnitude but may have large extent. We shall show how to calculate the effects of strong localized perturbations on the solutions of elliptic PDE problems and reaction-diffusion systems.

The examples of strong localized perturbations that we will consider are the removal of a small subdomain from the domain of a problem with the imposition of a boundary condition on the boundary of the resulting hole, a large alteration of the boundary condition on a small region of the boundary of the domain, a large but localized change in the coefficients of the differential operator, and nonlinear reaction diffusion problems where the nonlinearity is effectively localized in the domain.

Strong localized perturbations are singular perturbations in the sense that they produce large changes in the solutions of the problems in which they occur. However, these large changes are themselves localized. Consequently, the perturbed solutions can be constructed by the method of matched asymptotic expansions. An inner expansion can describe the large changes in the solution in a neighborhood of the strong perturbation. An outer expansion, valid in the region away from the strong perturbation can account for the relatively small effects that the perturbation produces there. These two expansions can be matched to determine the undetermined coefficients in both of them.

For strong localized perturbations in a 2-D domain, the asymptotic expansion of the solution often leads to infinite logarithmic series in powers of $\nu = -1/\log \varepsilon$, where ε is a small positive parameter, it is well-known that this method may be of only limited practical use in approximating the exact solution accurately. This difficulty stems from the fact that $\nu \to 0$ very slowly as ε decreases. Therefore, unless many coefficients in the infinite logarithmic series can be obtained analytically, the resulting low order truncation of this series will typically not be very accurate unless ε is very small. Singular perturbation problems involving infinite logarithmic expansions arise in many areas of application in two-dimensional spatial domains, including; low Reynolds number fluid flow past cylindrical bodies, eigenvalue problems in perforated domains, the calculation of the mean first passage time for Brownian motion in a domain with small traps, etc.

One primary goal of these notes is to highlight how a common analytical framework can be used to treat a wide range of problems with strong localized perturbations arising from different areas of application. There are some workshop problems that supplement the material presented, and which should be attempted by the reader. The solutions to these problems are given in the Appendices.

2 Strong Localized Perturbations in 3-D

We first recall a few basic results from potential theory. Suppose that $\Delta u - k^2 u = \delta(x - x_0)$ with $x \in \Omega \in \mathbb{R}^3$ and $k \geq 0$ a constant. Then,

$$u \sim \frac{1}{4\pi|x - x_0|} \quad \text{as} \quad x \to x_0 \,. \tag{2.1}$$

To derive this simple result, we introduce a small sphere of radius δ about x_0 so that $\Omega_\delta = \{x| \, |x - x_0| \leq \delta\}$. Then we define $r = |x - x_0|$, and we look for a local radially symmetric solution to

$$\Delta u - k^2 u = u_{rr} + \frac{2}{r} u_r - k^2 u = 0 \,,$$

that has a singularity at $r = 0$. We get $u = Ar^{-1}e^{-kr}$ for some constant A. Upon applying the divergence theorem,

$$\int_{\Omega_\delta} \Delta u \, dx - k^2 \int_{\Omega_\delta} u \, dx = \int_{\Omega_\delta} \delta(x - x_0) \, dx = 1 \,,$$

$$\int_{\partial\Omega_\delta} \nabla u \cdot n \, dS - k^2 \int_{\Omega_\delta} u \, dx = 4\pi \left(r^2 \frac{\partial u}{\partial r}\Big|_{r=\delta} \right) - k^2 \int_{\Omega_\delta} u \, dx = 1 \,.$$

Then, by substituting $u = Ar^{-1}e^{-kr}$ into the formula above, and taking the limit as $\delta \to 0$, we obtain $A = -1/4\pi$, which yields (2.1).

Therefore, if we want to solve in $\mathbb{R}^3$ the problem

$$\Delta u = 0 \,, \qquad x \in \Omega \backslash \{x_0\} \,,$$

$$u = 0 \qquad x \in \partial\Omega \,; \qquad u \sim \frac{A}{|x - x_0|} \qquad x \to x_0 \,,$$

we use the formal correspondence $-\frac{1}{4\pi|x-x_0|} \to \delta(x - x_0)$ to get $\frac{A}{|x-x_0|} \to -4\pi A\delta(x - x_0)$. Thus, the problem above becomes

$$\Delta u = -4\pi A \delta(x - x_0) \,, \qquad x \in \Omega \,; \qquad u = 0 \,, \qquad x \in \partial\Omega \,.$$

2.1 Eigenvalue Asymptotics in $\mathbb{R}^3$

Let Ω be a 3-D bounded domain with a hole of "radius" $\mathcal{O}(\epsilon)$, that is removed from Ω. We consider,

$$\begin{cases} \Delta u + \lambda u = 0 & \text{for } x \in \Omega \backslash \Omega_\epsilon \\ u = 0 & \text{for } x \in \partial\Omega \\ u = 0 & \text{for } x \in \partial\Omega_\epsilon \\ \int_{\Omega \backslash \Omega_\epsilon} u^2 \, dx = 1 \,. \end{cases} \tag{2.2}$$

We assume that Ω_ϵ shrinks to a point x_0 as $\epsilon \to 0$. For instance, Ω_ϵ could be the sphere $|x - x_0| \le \epsilon$, but more generally we will allow for holes of arbitrary shape. Then the unperturbed problem is

$$\begin{cases} \Delta\phi + \mu\phi = 0 & \text{for } x \in \Omega \\ \phi = 0 & \text{for } x \in \partial\Omega \\ \int_\Omega \phi^2 \, dx = 1 \, . \end{cases} \tag{2.3}$$

This problem has the eigenpairs $\phi_j(x)$, μ_j for $j = 0, 1, ...$ with the orthogonality property $\int_\Omega \phi_j \phi_k \, \mathrm{d}x = 0$ for $j \neq k$, and $\phi_0(x) > 0$ for $x \in \Omega$.

We now look for an eigenpair of (2.2) near the principal eigenpair $\phi_0(x)$, μ_0. We proceed by the method of matched asymptotic expansions. We first expand the eigenvalue for (2.2) as

$$\lambda \sim \mu_0 + \nu(\epsilon)\lambda_1 + \cdots \, ,$$

where $\nu(\epsilon) \to 0$ as $\varepsilon \to 0$ is some gauge function to be determined.

In the outer region away from the hole, we expand

$$u = \phi_0(x) + \nu(\epsilon) u_1 + \cdots \, .$$

Now since $\Omega_\epsilon \to \{x_0\}$ as $\epsilon \to 0$, then u_1 satisfies

$$\begin{cases} \Delta u_1 + \mu_0 u_1 = -\lambda_1 \phi_0 & \text{for } x \in \Omega \backslash \{x_0\} \\ u_1 = 0 & \text{for } x \in \partial\Omega \\ \int_\Omega u_1 \phi_0 \, \mathrm{d}x = 0 \, . \end{cases} \tag{2.4}$$

Now we construct an inner expansion near the hole. We let $y = \varepsilon^{-1}(x - x_0)$ and we define $v(y; \epsilon) = u(x_0 + \epsilon y)$. Then, $v(y)$ satisfies

$$\begin{cases} \Delta_y v + \lambda \epsilon^2 v = 0 & \text{for } x \notin \Omega_0 \\ v = 0 & \text{for } x \in \partial\Omega_0 \, . \end{cases} \tag{2.5}$$

Here $\Omega_0 = \varepsilon^{-1}\Omega_\epsilon$ is the magnified hole. Then, we expand $v = v_0 + \nu(\epsilon) v_1 + \cdots$, to obtain that v_0 satisfies

$$\begin{cases} \Delta_y v_0 = 0 & \text{for } y \notin \Omega \\ v_0 = 0 & \text{for } y \in \partial\Omega \\ v_0 \to \phi_0(x_0) & \text{as } |y| \to \infty \, . \end{cases} \tag{2.6}$$

The matching condition between the outer and inner solutions is that as $x \to x_0$ the outer expansion must agree with the far-field behavior as $|y| \to \infty$ of the inner expansion. We write this formally as

$$\phi_0(x) + \nu(\epsilon) u_1 + \cdots \sim v_0 + \nu(\epsilon) v_1 + \cdots \, , \quad \text{as } x \to x_0 \text{ and } |y| \to \infty \, . \tag{2.7}$$

Now we write the solution to (2.6) as

$$v_0 = \phi_0(x_0) \left(1 - v_c(y)\right) \, , \tag{2.8}$$

Trap Shape $\Omega_0 = \varepsilon^{-1}\Omega_\varepsilon$	Capacitance C
sphere of radius a	$C = a$
hemisphere of radius a	$C = 2a\left(1 - \frac{1}{\sqrt{3}}\right)$
flat disk of radius a	$C = \frac{2a}{\pi}$
prolate spheroid with semi-major and minor axes a, b	$C = \frac{\sqrt{a^2-b^2}}{\cosh^{-1}(a/b)}$
oblate spheroid with semi-major and minor axes a, b	$C = \frac{\sqrt{a^2-b^2}}{\cos^{-1}(b/a)}$
ellipsoid with axes a, b, and c	$C = 2\left(\int_0^\infty (a^2+\eta)^{-1/2}(b^2+\eta)^{-1/2}(c^2+\eta)^{-1/2}\, d\eta\right)^{-1}$

Table 1. Capacitance C of some simple trap shapes, defined from the solution to (2.9).

where $v_c(y)$ satisfies

$$\begin{cases} \Delta_y v_c = 0 & \text{for } y \notin \Omega_0 \\ v_c = 1 & \text{for } y \in \partial\Omega_0 \\ v_c \to 0 & \text{as } |y| \to \infty\,. \end{cases} \tag{2.9 a}$$

Except for a few simple shapes Ω_0, the solution for v_c cannot be found in closed form. However, it does have the well-known far-field asymptotic behavior

$$v_c \sim \frac{C}{|y|} + \mathcal{O}\left(|y|^{-2}\right) + \cdots\,, \qquad \text{as } |y| \to \infty\,, \tag{2.9 b}$$

where $C > 0$ is called the electrostatic capacitance of Ω_0.

As a remark, for the special case of a spherical trap of radius ε, then $\Omega_\epsilon = \{x \mid |x - x_0| \le \epsilon\}$ and $\Omega_0 = \{y \mid |y| \le 1\}$. We let $r = |y|$ so that in $\mathbb{R}^3$, $v_c = v_c(r)$ satisfies

$$\begin{cases} v_c'' + \frac{2}{r} v_c' = 0 & \text{for } r \ge 1 \\ v_c = 1 & \text{for } r = 1. \end{cases}$$

Then, $v_c = \frac{1}{r}$ for $r \ge 1$, so that $C = 1$.

The capacitance C, defined in (2.9), has two key properties. Firstly, it is invariant under rotations of the trap shape. Secondly, with respect to all trap shapes Ω_ε in of the same volume, C is minimized for a spherical-shaped trap (cf. [**72**]). Although C must in general be calculated numerically from (2.9) when Ω_ε has an arbitrary shape, it is known analytically for some simple shapes, as summarized in Table 1. The capacitance C is also known in a few other situations. For instance, for the case of two overlapping identical spheres of radius εa that intersect at exterior angle ψ, with $0 < \psi < \pi$, then C is given by (cf. [**25**])

$$C = 2\,a\,\sin\left(\frac{\psi}{2}\right)\int_0^\infty \left[1 - \tanh(\pi\tau)\tanh\left(\frac{\psi\tau}{2}\right)\right] d\tau\,. \tag{2.10}$$

For $\psi \to 0$, (2.10) reduces to the well-known result $C = 2a\log 2$ for the capacitance of two touching spheres.

Now we return to v_0 and write its far-field behavior as

$$v_0 \sim \phi(x_0)\left(1 - \frac{C}{|y|} + \cdots\right)\,, \quad \text{as} \quad |y| \to \infty\,.$$

We let $y = \varepsilon^{-1}(x - x_0)$ and use the matching condition of (2.7) to obtain

$$\phi_0(x_0) + \nu(\epsilon)u_1 \sim \phi_0(x_0) - \phi_0(x_0)\frac{\epsilon C}{|x - x_0|} + \cdots\,, \quad \text{as } x \to x_0\,.$$

This determines both the gauge function $\nu(\varepsilon)$ and the singularity behavior of u_1 as $x \to x_0$ as

$$\nu(\epsilon) = \epsilon\,, \qquad u_1 \to -\phi_0(x_0)\frac{C}{|x - x_0|}\,, \quad \text{as} \quad x \to x_0\,.$$

We then return to (2.4) and write this problem as

$$\begin{cases} \Delta u_1 + \mu_0 u_1 = -\lambda_1 \phi_0 & \text{for } x \in \Omega\backslash\{x_0\} \\ u_1 = 0 & \text{for } x \in \partial\Omega \\ u_1 \to -\phi_0(x_0)\frac{C}{|x-x_0|} & \text{as } x \to x_0 \\ \int_\Omega u_1\phi_0\,dx = 0\,. \end{cases}$$

Since $\frac{-1}{4\pi|x-x_0|} \to \delta(x - x_0)$, this problem is equivalent to

$$\begin{cases} Lu := \Delta u_1 + \mu_0 u_1 = -\lambda_1\phi_0 + 4\pi C\phi_0(x_0)\delta(x - x_0) & \text{in } \Omega \\ u_1 = 0 & \text{on } \partial\Omega\,. \end{cases}$$

We integrate Lu over Ω and use the Green's second identity to get

$$\int_\Omega (\phi_0 Lu_1 - u_1 L\phi_0)\ \mathrm{d}x = \int_{\partial\Omega} (\phi_0\partial_n u_1 - u_1\partial_n\phi_0)\,dS\,.$$

Since $\phi_0 = u_1 = 0$ on $\partial\Omega$, and $L\phi_0 = 0$, we obtain

$$0 = \int_\Omega \phi_0 Lu_1\,dx = \int_\Omega \phi_0(-\lambda_1\phi_0 + 4\pi C\phi_0(x_0)\delta(x - x_0))\,dx\,,$$

which determines λ_1 as $\lambda_1 = \frac{4\pi C[\phi_0(x_0)]^2}{\int_\Omega \phi_0^2 dx}$.

In summary with $\nu(\epsilon) = \epsilon$, we obtain the following two-term result for the expansion of the principal eigenvalue:

$$\lambda \sim \mu_0 + \epsilon\lambda_1 + \cdots\,, \qquad \lambda_1 = \frac{4\pi C[\phi_0(x_0)]^2}{\int_\Omega \phi_0^2\,dx}\,. \tag{2.11}$$

Remarks:

(1) If there are N small holes then we obtain

$$\lambda \sim \mu_0 + 4\pi\epsilon\sum_{j=1}^N C_j\frac{[\phi_0(x_j)]^2}{\int_\Omega \phi_0^2\,dx} + \cdots\,,$$

where C_j is the capacitance of the j^{th} hole.

(2) Let us assume that $u = 0$ on $\partial\Omega$ is replaced by the no-flux condition $\partial_n u = 0$ on $\partial\Omega$. Then,

$$\begin{cases} \Delta\phi + \mu\phi = 0 & \text{for } x \in \Omega \\ \partial_n\phi = 0 & \text{for } x \in \partial\Omega \\ \int_\Omega \phi^2\,dx = 1\,, \end{cases}$$

has the principal eigenpair $\mu_0 = 0$ and $\phi_0 = \frac{1}{|\Omega|^{1/2}}$, where $|\Omega|$ is the volume of Ω. In this case, we can readily calculate that $\lambda \sim \frac{4\pi\epsilon C}{|\Omega|}$, so that this leading-order term is independent of the location of the hole. We elaborate more on this case below in §2.3, as it is directly relevant to calculating the mean first passage time for diffusion inside a 3-D domain with absorbing traps inside the domain. A key issue below in §2.3 is to calculate higher-order terms in this expansion that reflect the location of the traps inside the domain.

Consider the special case of two concentric spheres with an inner sphere of small radius. The radially symmetric eigenfunctions, under Dirichlet conditions, satisfy

$$\begin{cases} u_{rr} + \frac{2}{r} u_r + \lambda u = 0 & \text{for } \epsilon < r < 1\,, \\ u(1) = 0\,, \quad u(\epsilon) = 0\,. \end{cases}$$

The exact eigenfunction is $u = r^{-1} \sin\left(\sqrt{\lambda}(r-\epsilon)\right)$. By satisfying $u(1) = 0$, we get $\sqrt{\lambda}(1-\epsilon) = \pi$, which yields $\lambda = \frac{\pi^2}{(1-\epsilon)^2} \sim \pi^2(1 + 2\epsilon + \cdots)$. Hence, $\lambda \sim \pi^2 + 2\epsilon\pi^2 + \cdots$.

Now use the asymptotic formula given in (2.11). In (2.11), we set $\mu_0 = \pi^2$, $\phi_0 = r^{-1}\sin(\pi r)$, so that $\phi_0(0) = \lim_{r\to 0} \frac{\sin(\pi r)}{r} = \pi$. In addition, $\int_\Omega \phi_0^2\, dx = 4\pi \int_0^1 \left(r^{-2}\sin^2(\pi r)\right) r^2\, dr = 2\pi$. Then (2.11) with $C = 1$ yields $\lambda \sim \pi^2 + 2\epsilon\pi^2 + \cdots$, in agreement with the expansion of the exact eigenvalue relation as shown above.

2.2 Narrow Capture Problem

Our next class of model problems to exhibit the asymptotic technique of treating localized traps is to construct an asymptotic solution in $\mathbf{R}^3$ to the following problem:

$$\begin{cases} \Delta u = M(x) & \text{for } x \in \Omega \backslash \cup_{j=1}^N \Omega_{\epsilon_j} \\ u = \alpha_j & \text{for } x \in \partial\Omega_{\epsilon_j}\,, \ \ j = 1, \ldots, N \\ u = 0 & \text{for } x \in \partial\Omega\,. \end{cases}$$

Here Ω_{ϵ_j} is a hole of "radius" ϵ with $\Omega_{\epsilon_j} \to \{x_j\}$ as $\epsilon \to 0$ for $j = 1, \ldots, N$. We assume that $x_j \in \Omega$, so that for $\varepsilon \to 0$ each hole is contained inside the domain.

In the outer region we expand

$$u = u_0 + \epsilon u_1 + \cdots\,,$$

where u_0 is the unperturbed solution in the absence of any holes, and satisfies

$$\begin{cases} \Delta u_0 = M(x) & \text{for } x \in \Omega \\ u_0 = 0 & \text{for } x \in \partial\Omega\,. \end{cases}$$

In addition, u_1 satisfies

$$\begin{cases} \Delta u_1 = 0 & \text{for } x \in \Omega \backslash \{x_1, \ldots, x_N\} \\ u_1 = 0 & \text{for } x \in \partial\Omega \\ u_1 \text{ singular} & \text{as } x \to x_j\,, \ j = 1, \ldots, N\,. \end{cases}$$

Now in the inner region near $x = x_j$ we write $y = \epsilon^{-1}(x - x_j)$ and $v(y;\epsilon) = u(x_j + \epsilon y, \epsilon) = v_0(y) + \cdots$. The matching condition yields that $v_0 \to u_0(x_j)$ as $|y| \to \infty$ so that

$$\begin{cases} \Delta_y v_0 = 0 & \text{for } y \notin \Omega_j = \varepsilon^{-1}\Omega_{\epsilon_j} \\ v_0 = \alpha_j & \text{for } x \in \partial\Omega_j \\ v_0 \to u_0(x_j) & \text{as } |y| \to \infty\,. \end{cases}$$

The solution is decomposed as

$$v_0 = u_0(x_j) + (\alpha_j - u_0(x_j))\, v_c(y)\,,$$

where $v_c(y)$ satisfies

$$\begin{cases} \Delta_y v_c = 0 & \text{for } y \notin \Omega_j \\ v_c = 1 & \text{for } y \in \Omega_j \\ v_c \sim \frac{C_j}{|y|} & \text{as } |y| \to \infty\ . \end{cases}$$

Here C_j is the capacitance of the j^{th} hole. This yields the far-field behavior

$$v_0 \sim u_0(x_j) + (\alpha_j - u_0(x_j))\, \frac{C_j}{|y|}\,, \quad \text{as} \quad |y| \to \infty\,.$$

Now the matching condition is simply

$$\underbrace{u_0(x_j) + \varepsilon(x - x_j)\cdot \nabla_x u_0(x_j) + \epsilon u_1}_{x \to x_j} + \cdots \sim u_0(x_j) + (\alpha_j - u_0(x_j))\, \frac{\epsilon C_j}{|x - x_j|} + \varepsilon v_1 + \cdots\,. \tag{2.12}$$

This yields that

$$u_1 \sim (\alpha_j - u_0(x_j))\, \frac{C_j}{|x - x_j|} \quad \text{as} \quad x \to x_j\,.$$

We remark that the gradient term on the left-hand side of (2.12) gives the far-field behavior of the v_1 term, and this would be the starting point to obtain a higher-order approximation.

Therefore, the problem for u_1 is simply

$$\begin{cases} \Delta u_1 = -4\pi \sum_{j=1}^{N} (\alpha_j - u_0(x_j))\ C_j \delta(x - x_j)\,, & \text{for } x \in \Omega \\ u_1 = 0 & \text{for } x \in \partial\Omega\,. \end{cases}$$

The solution is given by

$$u_1 = -4\pi \sum_{j=1}^{N} (\alpha_j - u_0(x_j))\ C_j\, G(x; x_j)\,,$$

where $G(x; x_j)$ is the Dirichlet Green's function satisfying

$$\begin{cases} \Delta G = \delta(x - x_j) & \text{for } x \in \Omega \\ G = 0 & \text{for } x \in \partial\Omega\,. \end{cases}$$

Now consider the corresponding Neumann problem in $\Omega \in \mathbf{R}^3$ given by

$$\begin{cases} \Delta u = M(x) & \text{for } x \in \Omega \backslash \cup_{j=1}^{N} \Omega_{\epsilon_j} \\ \partial_n u = 0 & \text{for } x \in \partial\Omega \\ u = \alpha_j & \text{for } x \in \partial\Omega_{\epsilon_j},\ j = 1, \ldots, N\,. \end{cases} \tag{2.13}$$

We assume for simplicity below that $\Omega_{\epsilon_j} = \{x |\, |x - x_j| = \epsilon r_j\}$ so that we have N-small spheres of radius ϵr_j. This simplification will allow us to readily calculate a two-term expansion for the solution.

Remarks:

(1) We cannot expand $u = u_0 + \epsilon u_1 + \cdots$ since

$$\begin{cases} \Delta u_0 = M(x) & \text{for } x \in \Omega \\ \partial_n u_0 = 0 & \text{for } x \in \partial\Omega\,, \end{cases}$$

has no solution in general unless $\int_\Omega M(x)\,dx = 0$.

(2) To identify the difficulty with this naive expansion, we recall that the underlying spectral problem given by

$$\begin{cases} \Delta\phi + \lambda\phi = 0 & \text{for } x \in \Omega\backslash \cup_{j=1}^N \Omega_{\epsilon_j} \\ \partial_n \phi = 0 & \text{for } x \in \partial\Omega \\ \phi = 0 & \text{for } x \in \partial\Omega_{\epsilon_j}\,, \ j = 1, \ldots, N\,, \end{cases}$$

has a principal eigenvalue (see the earlier example) with estimate

$$\lambda \sim \frac{4\pi\epsilon}{|\Omega|} \sum_{j=1}^N C_j = \mathcal{O}(\varepsilon)\,.$$

Thus, the Neumann BVP is "almost" not solvable. The principal eigenvalue estimate $\lambda = \mathcal{O}(\epsilon)$ suggests that the expansion for u should be $u = \varepsilon^{-1}u_0 + u_1 + \epsilon u_2 + \cdots$.

Notice that in the j^{th} inner region, the leading-order inner solution satisfies

$$\begin{cases} \Delta_y v_c = 0 & |y| \geq r_j \\ v_c = 1 & |y| = r_j\,, \end{cases}$$

with $v_c \sim C_j/|y|$ as $|y| \to \infty$. The exact solution is $v_c = r_j/|y|$, so that $C_j = r_j$.

(3) Consider the special case of this problem posed in a concentric annulus formulated as

$$\begin{cases} \Delta u = M & \text{for } \epsilon < r < 1 \\ u_r = 0 & \text{for } r = 1 \\ u = 1 & \text{for } r = \epsilon\,, \end{cases}$$

where M is assumed to be a constant, independent of x. The exact solution is readily found to be

$$u = \frac{M}{6}(r^2 - \epsilon^2) + \frac{M}{3}(\frac{1}{r} - \frac{1}{\epsilon}) + 1\,.$$

Notice that in the outer region, the exact solution gives

$$u = \frac{u_0}{\epsilon} + u_1 + \cdots\,,$$

while in the inner region with $r = \mathcal{O}(\varepsilon)$, we have

$$v = \frac{v_0}{\epsilon} + v_1 + \cdots\,.$$

We then return to (2.13). In the outer region, we expand

$$u = \frac{u_0}{\epsilon} + u_1 + \epsilon u_2 + \cdots\,.$$

We obtain that $\Delta u_0 = 0$ with $\partial_n u_0 = 0$ on $\partial\Omega$, and so $u_0 = \mu$ where μ is a constant. The problem for u_1 is

$$\begin{cases} \Delta u_1 = M(x) & \text{for } x \in \Omega\backslash\{x_1, \ldots, x_N\} \\ \partial_n u_1 = 0 & \text{for } x \in \partial\Omega \\ u_1 \text{ singular} & \text{as } x \to x_j\,, \ \ j = 1, \ldots, N\,, \end{cases}$$

while u_2 satisfies

$$\begin{cases} \Delta u_2 = 0 & \text{for } x \in \Omega \backslash \{x_1, \ldots, x_N\} \\ \partial_n u_2 = 0 & \text{for } x \in \partial\Omega \\ u_2 \text{ singular} & \text{as } x \to x_j\,, \;\; j = 1, \ldots, N\,. \end{cases}$$

Now in the inner region we let $y = \epsilon^{-1}(x - x_j)$, and we expand the inner solution as

$$v = \frac{v_0}{\epsilon} + v_1 + \epsilon v_2 + \cdots\,.$$

We obtain, upon using the matching condition $v_0 \to u_0$ as $|y| \to \infty$ that

$$\begin{cases} \Delta_y v_0 = 0 & \text{for } |y| \geq r_j \\ v_0 = 0 & \text{for } |y| = r_j \\ v_0 \to \mu & \text{as } |y| \to \infty\,. \end{cases}$$

The solution is written as $v_0 = \mu(1 - v_c)$, where $v_c = C_j/|y|$ and $C_j = r_j$. The matching condition for $x \to x_j$ becomes

$$\underbrace{\frac{\mu}{\epsilon} + u_1 + \epsilon u_2 + \cdots}_{x \to x_j} \sim \underbrace{\frac{v_0}{\epsilon} + v_1 + \cdots}_{y \to \infty} = \frac{\mu}{\epsilon}\left(1 - \frac{C_j}{|x - x_j|}\epsilon\right) + v_1 + \cdots\,.$$

Therefore, we obtain

$$u_1 \to -\frac{\mu C_j}{|x - x_j|}\,, \quad \text{as} \quad x \to x_j\,.$$

The problem for u_1 is simply

$$\begin{cases} \Delta u_1 = M(x) & \text{for } x \in \Omega \backslash \{x_1, \ldots, x_N\} \\ \partial_n u_1 = 0 & \text{for } x \in \partial\Omega \\ u_1 \sim -\frac{\mu C_j}{|x - x_j|} & \text{as } x \to x_j\,, \;\; j = 1, \ldots, N\,, \end{cases}$$

which is equivalent to

$$\begin{cases} \Delta u_1 = M(x) + 4\pi\mu \sum_{j=1}^N C_j \delta(x - x_j) & \text{for } x \in \Omega \\ \partial_n u_1 = 0 & \text{for } x \in \partial\Omega\,. \end{cases}$$

Upon using the divergence theorem, we obtain that

$$\int_\Omega M(x)\, dx + 4\pi\mu \sum_{j=1}^N C_j = 0\,.$$

This yields the leading-order outer solution as

$$u \sim \frac{\mu}{\epsilon}\,, \qquad \text{where} \quad \mu = -\frac{1}{4\pi} \frac{\int_\Omega M(x)\, dx}{\sum_{j=1}^N C_j}\,.$$

Now we proceed to one higher order in the asymptotic construction. To do so, we must solve for u_1 explicitly. This is done by introducing the Neumann Green's function $G(x; x_j)$ defined uniquely by the solution to

$$\Delta G = \frac{1}{|\Omega|} - \delta(x - x_j)\,, \quad x \in \Omega\,, \tag{2.14 a}$$

$$\partial_n G = 0\,, \quad x \in \partial\Omega\,, \tag{2.14 b}$$

$$\int_\Omega G\, dx = 0\,. \tag{2.14 c}$$

We notice that $G(x;x_j)$ exists since $\int_\Omega \left(\frac{1}{|\Omega|} - \delta(x-x_j)\right)\, dx = 0$, and the condition $\int_\Omega G\, dx = 0$ specifies G uniquely. In addition, we can decompose $G(x;x_j)$ as

$$G(x;x_j) = \frac{1}{4\pi|x-x_j|} + R(x;x_j)\,, \tag{2.14 d}$$

where $R(x;x_j)$ is the regular (smooth) part of the Neumann Green's function. Therefore, as $x \to x_j$ we obtain

$$G(x;x_j) \sim \frac{1}{4\pi|x-x_j|} + R_j + o(1)\,, \quad \text{as} \quad x \to x_j\,; \qquad R_j \equiv R(x_j;x_j)\,.$$

Now we write the problem for u_1 as

$$\begin{cases} \Delta u_1 = \left(M(x) - \frac{1}{|\Omega|}\int_\Omega M\, dx\right) + \left(\frac{1}{|\Omega|}\int_\Omega M(x)\, dx + 4\pi\mu \sum_{j=1}^N C_j \delta(x-x_j)\right) & \text{for } x \in \Omega \\ \partial_n u_1 = 0 & \text{for } x \in \partial\Omega\,. \end{cases}$$

We decompose the solution to this problem in the form

$$u_1 = u_{1_p} - 4\pi\mu \sum_{j=1}^N C_j G(x;x_i) + \bar{u}_1\,. \tag{2.15}$$

Here $\bar{u}_1$ is a constant, while u_{1_p} is the unique solution to

$$\begin{cases} \Delta u_{1_p} = M(x) - \frac{1}{|\Omega|}\int M\, dx & \text{for } x \in \Omega \\ \partial_n u_{1_p} = 0 & \text{for } x \in \partial\Omega \\ \int_\Omega u_{1_p}\, dx = 0\,. \end{cases}$$

A simple calculation shows that

$$\Delta[-4\pi\mu \sum_{i=1}^N C_i G] = -4\pi\mu \sum_{i=1}^N C_i \left(\frac{1}{|\Omega|} - \delta(x-x_i)\right) = 4\pi\mu \sum_{i=1}^N C_i \delta(x-x_i) + \frac{1}{|\Omega|}\int_\Omega M(x)\, dx\,.$$

Notice that u_{1_p} is uniquely determined. In addition, since $\int_\Omega u_{1_p}\, dx = 0$ and $\int_\Omega G(x;x_j)\, dx = 0$, it follows that $\int_\Omega u_1\, dx = \bar{u}_1|\Omega|$. Therefore, $\bar{u}_1$ in (2.15) has the interpretation that it is the spatial average of u_1, i.e. $\bar{u}_1 = \frac{1}{|\Omega|}\int_\Omega u_1\, dx$.

Now we expand the solution in (2.15) as $x \to x_j$ for each $j = 1, \ldots, N$ to obtain

$$u_1 \sim u_{1_p}(x_j) - 4\pi\mu\left(\sum_{i\neq j}^N C_i G(x_j;x_i) + C_j\left(\frac{1}{4\pi|x-x_j|} + R_j\right)\right) + \bar{u}_1\,.$$

We write this expression as

$$u_1 \sim B_j + \bar{u}_1 - \frac{\mu C_j}{|x-x_j|}\,, \qquad \text{as} \qquad x \to x_j\,,$$

where B_j is defined by

$$B_j = u_{1_p}(x_j) - 4\pi\mu\left(C_j R_j + \sum_{i\neq j}^N C_i G(x_j;x_i)\right)\,.$$

Then, the matching condition is

$$\frac{\mu}{\epsilon} + u_1 + \epsilon u_2 + \cdots \sim \frac{v_0}{\epsilon} + v_1 + \cdots\,.$$

Writing this condition out in detail we have

$$\frac{\mu}{\epsilon} + \bar{u}_1 + B_j - \frac{\mu C_j}{|x-x_j|} + \epsilon u_2 \sim \frac{\mu}{\epsilon}\left(1 - \frac{C_j \epsilon}{|x-x_j|}\right) + v_1\,.$$

This implies that for each $j = 1, \ldots, N$, v_1 must satisfy

$$\begin{cases} \Delta_y v_1 = 0 & \text{for } |y| \geq r_j \\ v_1 = \alpha_j & \text{for } |y| = r_j \\ v_1 \sim \bar{u}_1 + B_j & \text{as } |y| \to \infty\,. \end{cases}$$

The solution is given explicitly by

$$v_1 = (\bar{u}_1 + B_j) - [(\bar{u}_1 + B_j) - \alpha_j]v_c\,, \qquad v_c = C_j/|y|\,, \quad C_j = r_j\,.$$

Therefore, $v_1 \sim (\bar{u}_1 + B_j) - [(\bar{u}_1 + B_j) - \alpha_j]\frac{C_j}{|y|}$ as $|y| \to \infty$. This implies from the matching condition that u_2 must satisfy

$$\begin{cases} \Delta u_2 = 0 & \text{for } x \in \Omega \backslash \{x_1, \ldots, x_N\} \\ \partial_n u_2 = 0 & \text{for } x \in \partial\Omega \\ u_2 \sim [\alpha_j - (\bar{u}_1 + B_j)]\frac{C_j}{|x - x_j|} & \text{as } x \to x_j \quad j = 1, \ldots, N\,. \end{cases}$$

Therefore, we can write the problem for u_2 as

$$\Delta u_2 = -4\pi \sum_{j=1}^{N} [\alpha_j - (\bar{u}_1 + B_j)]C_j \delta(x - x_j) \qquad x \in \Omega\,; \qquad \partial_n u_2 = 0\,, \quad \text{on} \quad \partial\Omega\,.$$

Finally, we determine $\bar{u}_1$ by the divergence theorem. We calculate

$$\sum_{j=1}^{N} [\alpha_j - (\bar{u}_1 + B_j)]C_j = 0\,,$$

so that

$$\bar{u}_1 = \frac{\sum_{j=1}^{N} (\alpha_j - B_j)C_j}{\sum_{j=1}^{N} C_j}\,. \tag{2.16 a}$$

where

$$B_j = u_{1_p}(x_j) - 4\pi\mu\left(C_j R_j + \sum_{i \neq j}^{N} C_i G(x_j; x_i)\right)\,. \tag{2.16 b}$$

In summary, a two-term outer expansion for (2.13) is given by

$$u \sim \frac{\mu}{\epsilon} + u_1 + \cdots\,, \quad \text{with} \quad \mu = -\frac{1}{4\pi}\frac{\int_\Omega M(x)\, dx}{\sum_{j=1}^{N} C_j}\,,$$

where u_1 is given by $u_1 = u_{1_p}(x) + \bar{u}_1 - 4\pi\mu\sum_{i=1}^{N} C_i G(x; x_i)$. Finally, the constant term $\bar{u}_1$ is given in (2.16).

We now show that our result agrees with the exact solution to the concentric annulus problem with M constant, formulated as

$$\begin{cases} \Delta u = M & \text{for } \epsilon < r < 1 \\ u_r = 0 & \text{for } r = 1 \\ u = 1 & \text{for } r = \epsilon \end{cases}$$

We recall that the exact solution is $u = \frac{M}{6}(r^2 - \epsilon^2) + \frac{M}{3}(\frac{1}{r} - \frac{1}{\epsilon}) + 1$.

To recover this result, we use in our asymptotic result that $j = 1, x_1 = 0, C_1 = 1, \alpha_1 = 1$ and $u_{1_p} = 0$ since M

constant. In addition, the Neumann Green's function for the unit sphere with a source point at the origin satisfies

$$\begin{cases} \Delta G = \frac{1}{|\Omega|} & \text{for } x \in \Omega \backslash \{0\} \\ G_r = 0 & \text{on } r = 1 \\ G \sim \frac{1}{4\pi r} + R_1 & \text{as } r \to 0 \\ \int G \, \mathrm{d}x = 0 \,. \end{cases}$$

A simple calculation gives

$$G = -\frac{9}{20\pi} + \frac{1}{4\pi r} + \frac{r^2}{8\pi} \,.$$

Now as $r \to 0$, then $G \sim \frac{1}{4\pi r} + R_1$, where we identify $R_1 = -\frac{9}{20\pi}$.

In our asymptotic result we must calculate μ, B_1, and $\bar{u}_1$. We obtain

$$\mu = -\frac{1}{4\pi C_1} \int_\Omega M \, dx = -\frac{M}{4\pi(1)} \left(\frac{4\pi}{3} \right) = -\frac{M}{3} \,, \qquad B_1 = -4\pi\mu C_1 R_1 = -4\pi(\frac{M}{3})(-\frac{9}{20\pi}) = -\frac{3M}{5\pi} \,.$$

This yields that

$$\bar{u}_1 = (\alpha_1 - B_1)\frac{C_1}{C_1} = (1 + \frac{3M}{5}) \,.$$

Then u_1 is given explicitly by

$$\begin{cases} u_1 = u_{1_p} + \bar{u}_1 - 4\pi\mu C_1 G = 1 + \frac{3M}{5} - 4\pi(-\frac{M}{3})[-\frac{9}{20\pi} + \frac{1}{4\pi r} + \frac{r^2}{8\pi}] \\ u_1 = 1 + \frac{4\pi}{3} M(\frac{1}{4\pi r} + \frac{r^2}{8\pi}) = 1 + \frac{M}{3r} + \frac{Mr^2}{6} \,. \end{cases}$$

Therefore to to second-order our asymptotic result is $u \sim \frac{\mu}{\epsilon} + u_1 + \cdots$, which yields $u \sim 1 + \frac{M}{3}(\frac{1}{r} - \frac{1}{\epsilon}) + \frac{Mr^2}{6}$. This agrees with the exact solution up to the terms of $\mathcal{O}(\epsilon^2)$.

2.3 An Eigenvalue Optimization Problem and the Mean First Passage Time

We now apply the asymptotic methodology to the problem of determining the mean first passage time (MFPT) for Brownian motion inside a three-dimensional domain with N localized traps. This section is motivated by the recent paper [**16**]. For a fixed trap volume fraction, which spatial arrangement of traps will minimize the average MFPT. Is the effect of fragmentation of the trap set significant? In other words, is there much difference in the MFPT when we replace N small traps by one larger "effective" trap that maintains the volume of the trap set? Such questions are relevant in biological cell signalling when one considers how to model the highly spatially heterogeneous cell cytoplasm.

The mathematical problem is formulated as follows: We consider an optimization problem for the principal eigenvalue of the Laplacian in a bounded three-dimensional domain with a reflecting boundary that is perturbed by the presence of N small traps in the interior of the domain. The perturbed eigenvalue problem is formulated as

$$\Delta u + \lambda u = 0 \,, \quad x \in \Omega \backslash \Omega_a \,; \qquad \int_{\Omega \backslash \Omega_a} u^2 \, dx = 1 \,, \tag{2.17 a}$$

$$\partial_n u = 0 \,, \quad x \in \partial\Omega \,, \tag{2.17 b}$$

$$u = 0 \,, \quad x \in \partial\Omega_a \equiv \cup_{j=1}^N \partial\Omega_{\varepsilon_j} \,. \tag{2.17 c}$$

Here Ω is the unperturbed domain, $\Omega_a \equiv \cup_{j=1}^N \Omega_{\varepsilon_j}$ is a collection of N small interior traps Ω_{ε_j}, for $j = 1, \ldots, N$, each of 'radius' $\mathcal{O}(\varepsilon) \ll 1$, and $\partial_n u$ is the outward normal derivative of u on $\partial\Omega$. We assume that $\Omega_{\varepsilon_j} \to x_j$ uniformly as $\varepsilon \to 0$, for $j = 1, \ldots, N$, and that the traps are well-separated in the sense that $\text{dist}(x_i, x_j) = \mathcal{O}(1)$ for $i \neq j$ and $\text{dist}(x_j, \partial\Omega) = \mathcal{O}(1)$ for $j = 1, \ldots, N$.

The primary motivation for considering (2.17) is its relationship to determining the mean first passage time (MFPT) for a Brownian particle wandering inside a three-dimensional domain that contains N localized absorbing traps. Denoting the trajectory of the Brownian particle by $X(t)$, the MFPT $v(x)$ is defined as the expectation value of the time τ taken for the Brownian particle to become absorbed somewhere in $\partial\Omega_a$ starting initially from $X(0) = x \in \Omega$, so that $v(x) = E[\tau \,|\, X(0) = x]$. The calculation of $v(x)$ becomes a narrow capture problem in the limit when the volume of the absorbing set $|\partial\Omega_a| = \mathcal{O}(\varepsilon^3)$ is asymptotically small, where $0 < \varepsilon \ll 1$ measures the dimensionless trap radius. Since the MFPT diverges as $\varepsilon \to 0$, the calculation of the MFPT $v(x)$ constitutes a singular perturbation problem. It is well-known (cf. [**29**], [**58**]) that the MFPT $v(x)$ satisfies a Poisson equation with mixed Dirichlet-Neumann boundary conditions, formulated as

$$\Delta v = -\frac{1}{D}\,, \quad x \in \Omega \backslash \Omega_a\,,\,, \tag{2.18 a}$$

$$\partial_n v = 0\,, \quad x \in \partial\Omega\,; \qquad v = 0\,, \qquad x \in \partial\Omega_a = \cup_{j=1}^{N} \partial\Omega_{\varepsilon_j}\,, \tag{2.18 b}$$

where D is the diffusivity of the underlying Brownian motion. With respect to a uniform distribution of initial points $x \in \Omega$ for the Brownian walk, the average MFPT, denoted by $\bar{v}$, is defined by

$$\bar{v} = \chi \equiv \frac{1}{|\Omega\backslash\Omega_a|} \int_{\Omega\backslash\Omega_a} v(x)\, dx\,, \tag{2.19}$$

where $|\Omega\backslash\Omega_a|$ is the volume of the trap-free domain.

The mean first passage time v is readily calculated by using the matched asymptotic approach of §2.1. Alternatively, v can be calculated by representing it as an eigenfunction expansion in terms of the normalized eigenfunctions ϕ_k and eigenvalues λ_k for $k \geq 1$ of (2.17). In the trap-free domain $\Omega_p = \Omega\backslash\Omega_a$, we readily derive that

$$v = \frac{1}{D} \left[\frac{\phi_1}{\lambda_1} \left(\int_{\Omega_p} \phi_1 \, dx \right) + \sum_{k=2}^{\infty} \frac{\phi_k}{\lambda_k} \left(\int_{\Omega_p} \phi_k \, dx \right) \right]. \tag{2.20}$$

For $\varepsilon \to 0$, the principal eigenpair λ_1, ϕ_1, are given in (2.22 a) and (2.22 c), respectively. They satisfy $\phi_1 \int_{\Omega_p} \phi_1\, dx = 1 + \mathcal{O}(\varepsilon^2)$ and $\lambda_1 = \mathcal{O}(\varepsilon)$. Next, we give a rough estimate of the asymptotic order of the infinite sum in (2.20). This infinite sum does converge for each fixed ε, since $\lambda_k = \mathcal{O}(k^2)$ as $k \to \infty$. However, for each fixed k with $k > 2$, we have that $\lambda_k = \lambda_{k0} + \mathcal{O}(\varepsilon)$ as $\varepsilon \to 0$, where $\lambda_{k0} > 0$ for $k \geq 2$ are the eigenvalues of the Laplacian in the trap-free unit sphere with homogeneous Neumann boundary condition. In addition, for each fixed k with $k \geq 2$, we have that $\int_{\Omega_p} \phi_k\, dx = \mathcal{O}(\varepsilon)$, due to the near orthogonality of ϕ_k and 1 as $\varepsilon \to 0$ when $k \geq 2$. In this way, for $\varepsilon \to 0$, the infinite sum in (2.20) contributes at most an $\mathcal{O}(\varepsilon)$ term, and consequently it can be neglected in comparison with the leading term in (2.20). In particular, one can readily show that the average MFPT $\bar{v}$ is given asymptotically for $\varepsilon \to 0$ in terms of the principal eigenvalue λ_1 by

$$\bar{v} = \chi \sim \frac{1}{D\lambda_1} + \mathcal{O}(\varepsilon)\,. \tag{2.21}$$

This narrow capture problem has wide applications in cellular signal transduction. In particular, in many cases a diffusing molecule must arrive at a localized signaling region within a cell before a signaling cascade can be initiated. Of primary importance then is to determine how quickly such a diffusing molecule can arrive at any one of these localized regions. Our narrow capture problem is closely related to the so-called narrow escape problem, related to the expected time required for a Brownian particle to escape from a confining bounded domain that has N localized windows on an otherwise reflecting boundary. The narrow escape problem has many applications in biophysical modeling (see [**4**], [**29**], [**62**], and the references therein). The narrow escape problem in both two- and three-dimensional confining domains has been studied with a variety of analytical methods in [**29**], [**66**], [**65**], [**30**], [**53**], and [**15**].

We let $\lambda(\varepsilon)$ denote the first eigenvalue of (2.17), with corresponding eigenfunction $u(x,\varepsilon)$. Clearly, $\lambda(\varepsilon) \to 0$ as $\varepsilon \to 0$. For $\varepsilon \to 0$, a simple calculation shows that $\lambda(\varepsilon)$ is related to the average MFPT χ by $\lambda(\varepsilon) \sim 1/(D\chi)$. One of the main objectives is to derive a two-term asymptotic expansion for $\lambda(\varepsilon)$ as $\varepsilon \to 0$. Such a two-term expansion not only provides a more accurate determination, when ε is not too small, of the principal eigenvalue and the corresponding average MFPT, it also provides an explicit formula showing how the locations of the traps within the domain influence these quantities. As explained in §2.1, we emphasize that the leading-order term in the expansion of $\lambda(\varepsilon)$ as $\varepsilon \to 0$ is independent of the locations of the traps. By examining the coefficient of the second-order term in the expansion of $\lambda(\varepsilon)$ we will formulate a discrete optimization problem for the spatial configuration $\{x_1, \ldots, x_N\}$ of the centers of the N traps of fixed given shapes that maximizes this principal eigenvalue $\lambda(\varepsilon)$, and correspondingly minimizes the average MFPT χ.

By using the method of matched asymptotic expansions in a similar way as for the simple model problem of §2.1, we readily obtain the following result of [**16**]:

Principal Result 2.1: *In the limit of small trap radius, $\varepsilon \to 0$, the principal eigenvalue $\lambda(\varepsilon)$ of (2.17) has the two-term asymptotic expansion*

$$\lambda(\varepsilon) \sim \frac{4\pi\varepsilon N}{|\Omega|}\bar{C} - \frac{16\pi^2\varepsilon^2}{|\Omega|} p_c(x_1, \ldots, x_N) \,. \tag{2.22 a}$$

Here $\bar{C} \equiv N^{-1}(C_1 + \ldots + C_N)$ and $p_c(x_1, \ldots, x_N)$ is the discrete sum defined in terms of the entries $\mathcal{G}_{i,j}$ of the Green's matrix $\mathcal{G}$ of (2.23) by

$$p_c(x_1, \ldots, x_N) \equiv c^T \mathcal{G} c = \sum_{i=1}^{N} \sum_{j=1}^{N} C_i C_j \mathcal{G}_{i,j} \,. \tag{2.22 b}$$

The corresponding eigenfunction u is given asymptotically in the outer region $|x - x_j| >> \mathcal{O}(\varepsilon)$ for $j = 1, \ldots, N$ by

$$u \sim \frac{1}{|\Omega|^{1/2}} - \frac{4\pi\varepsilon}{|\Omega|^{1/2}} \sum_{j=1}^{N} C_j G(x; x_j) + \mathcal{O}(\varepsilon^2) \,. \tag{2.22 c}$$

For $\varepsilon \ll 1$, the principal eigenvalue $\lambda(\varepsilon)$ is maximized when the trap configuration $\{x_1, \ldots, x_N\}$ is chosen to minimize $p_c(x_1, \ldots, x_N)$. For N identical traps with a common capacitance C, (2.22 a) reduces to

$$\lambda(\varepsilon) \sim \frac{4\pi\varepsilon N C}{|\Omega|}\left[1 - \frac{4\pi\varepsilon C}{N} p(x_1, \ldots, x_N)\right] \,, \qquad p(x_1, \ldots, x_N) \equiv \boldsymbol{e}^T \mathcal{G} \boldsymbol{e} = \sum_{i=1}^{N} \sum_{j=1}^{N} \mathcal{G}_{i,j} \,. \tag{2.22 d}$$

In this result, we have defined the capacitance vector c and the symmetric Neumann Green's matrix $\mathcal{G}$ by

$$\mathcal{G} \equiv \begin{pmatrix} R_{1,1} & G_{1,2} & \cdots & G_{1,N} \\ G_{2,1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & G_{N-1,N} \\ G_{N,1} & \cdots & G_{N,N-1} & R_{N,N} \end{pmatrix}, \qquad c \equiv \begin{pmatrix} C_1 \\ \vdots \\ C_N \end{pmatrix}. \tag{2.23}$$

Here C_j is the capacitance of the j^{th} trap defined in (2.9), and $G_{i,j} \equiv G(x_i; x_j)$ for $i \neq j$ is the Neumann Green's function of (2.14) with regular part $R_{j,j} \equiv R(x_j; x_j)$. At this stage, the reader should attempt the following problem:

Problem 2.1: *Derive Principal Result 2.1 by extending the calculation of the simple model problem of §2.1 to one higher order.*

The solution to this problem is given in Appendix A. The next result is for the average MFPT.

Principal Result 2.2 *In the limit $\varepsilon \to 0$ of small trap radius, the average mean first passage time $\bar{v}$, based on a uniform distribution of starting points for the Brownian motion, is given for $\varepsilon \to 0$ by $\bar{v} \sim |\Omega|^{-1} \int_\Omega v \, dx$, and is given explicitly by*

$$\bar{v} \sim \frac{1}{D\lambda_1} + \mathcal{O}(\varepsilon) = \frac{|\Omega|}{4\pi N \bar{C} D \varepsilon} \left[1 + \frac{4\pi\varepsilon}{N\bar{C}} p_c(x_1, \ldots, x_N) + \mathcal{O}(\varepsilon^2) \right]. \tag{2.24}$$

The derivation of this follows immediately by using the result for $\lambda(\varepsilon)$ in Principal Result 2.1 in (2.21).

We now optimize the coefficient of the second-order term in the asymptotic expansion of λ in (2.22 *d*) of Principal Result 2.1 for the special case when Ω is a sphere of radius one that contains N small identically-shaped traps of a common "radius" ε. To do so, we require the Neumann Green's function of (2.14) for the unit sphere as given explicitly by (see Appendix A of [**16**])

$$G(x;\xi) = \frac{1}{4\pi|x-\xi|} + \frac{1}{4\pi|x||x'-\xi|} + \frac{1}{4\pi} \log\left(\frac{2}{1 - |x||\xi|\cos\theta + |x||x'-\xi|} \right) + \frac{1}{6|\Omega|} \left(|x|^2 + |\xi|^2 \right) - \frac{7}{10\pi}, \tag{2.25 a}$$

where $|\Omega| = 4\pi/3$. Here $x' = x/|x|^2$ is the image point to x outside the unit sphere, and θ is the angle between ξ and x, i.e. $\cos\theta = x \cdot \xi / |x||\xi|$, where $\cdot$ denotes the dot product.

To calculate $R(\xi;\xi)$ from (2.25 *a*) we take the limit of $G(x,\xi)$ as $x \to \xi$ and extract the nonsingular part of the resulting expression. Setting $x = \xi$ and $\theta = 0$ in (2.25 *a*), we obtain $|x' - \xi| = -|\xi| + 1/|\xi|$, so that

$$R(\xi,\xi) = \frac{1}{4\pi\left(1 - |\xi|^2\right)} + \frac{1}{4\pi} \log\left(\frac{1}{1 - |\xi|^2} \right) + \frac{|\xi|^2}{4\pi} - \frac{7}{10\pi}. \tag{2.25 b}$$

Next, we compute optimal spatial arrangements $\{x_1, \ldots, x_N\}$ of $N \geq 2$ identically shaped traps inside the unit sphere that minimizes $p(x_1, \ldots, x_N)$ in (2.22 *d*), or equivalently maximizes the coefficient of the second-order term in ε in the asymptotic expansion of $\lambda(\varepsilon)$ given in (2.22 *d*). To simplify the computation, we will minimize the function $\mathcal{H}_{\text{ball}}$ defined in terms of p of (2.22 *d*) by

$$\mathcal{H}_{\text{ball}} \equiv \sum_{i=1}^{N} \sum_{j=1}^{N} \widetilde{\mathcal{G}}_{i,j} = \sum_{i=1}^{N} \sum_{j=1}^{N} \left((1 - \delta_{ij}) \widetilde{G}_{ij} + \delta_{ij} \widetilde{R}_{ii} \right), \qquad p(x_1, \ldots, x_N) = \frac{\mathcal{H}_{\text{ball}}}{4\pi} - \frac{7N^2}{10\pi}, \tag{2.26}$$

where $\delta_{ij} = 0$ if $i \neq j$ and $\delta_{jj} = 1$. Here we have defined $\widetilde{\mathcal{G}}_{i,j}$, $\widetilde{G}_{i,j}$ and $\widetilde{R}_{j,j}$ by $\widetilde{\mathcal{G}}_{i,j} = 4\pi(\mathcal{G}_{i,j} - B)$, $\widetilde{G}_{i,j} \equiv 4\pi(G_{i,j} - B)$, and $\widetilde{R}_{j,j} \equiv 4\pi(R_{j,j} - B)$, where $B = -7/(10\pi)$ and $G_{i,j}$ and $R_{j,j}$ are obtained from (2.25).

N	$\mathcal{H}_{\text{ball}}^{(a)}$	Spherical radii $r_1 = ... = r_N$	$\mathcal{H}_{\text{ball}}^{(b)}$	Spherical radii $r_2 = ... = r_N$ $(r_1 = 0)$
2	**7.2763**	0.429	9.0316	0.563
3	**18.5047**	0.516	20.3664	0.601
4	**34.5635**	0.564	36.8817	0.626
5	**56.2187**	0.595	58.1823	0.645
6	**82.6490**	0.618	85.0825	0.659
7	**115.016**	0.639	116.718	0.671
8	**152.349**	0.648	154.311	0.680
9	**195.131**	0.659	196.843	0.688
10	**243.373**	0.668	244.824	0.694
11	**297.282**	0.676	297.283	0.700
12	**355.920**	0.683	357.371	0.705
13	**420.950**	0.689	421.186	0.710
14	**491.011**	0.694	491.415	0.713
15	**566.649**	0.698	566.664	0.717
16	647.738	0.702	**647.489**	0.720
17	734.344	0.706	**733.765**	0.722
18	826.459	0.709	**825.556**	0.725
19	924.360	0.712	**922.855**	0.727
20	1027.379	0.715	**1025.94**	0.729

Table 2. Numerically computed minimal values of the discrete energy functions $\mathcal{H}_{\text{ball}}^{(a)}$ and $\mathcal{H}_{\text{ball}}^{(b)}$ for the optimal arrangement of N-traps within a unit sphere, as computed using the DSO method. The numerically computed minimum value of $\mathcal{H}_{\text{ball}}$ in (2.26) is shown in bold face.

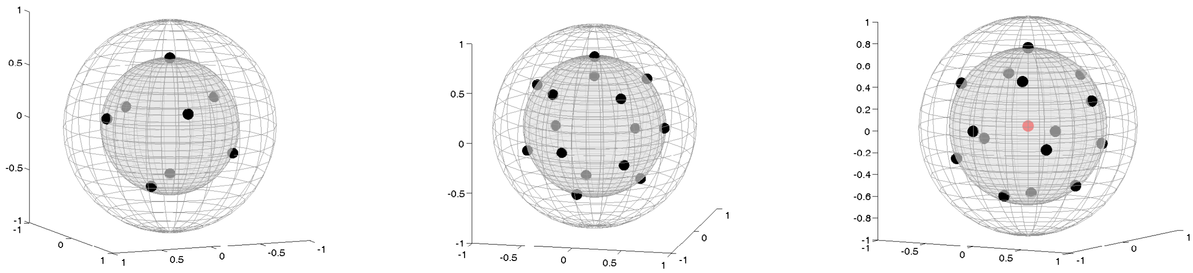
Various numerical methods for global optimization are available, including

(1) *The Extended Cutting Angle method (ECAM).* This deterministic global optimization technique is applicable to Lipschitz functions. Within the algorithm, a sequence of piecewise linear lower approximations to the objective function is constructed. The sequence of the corresponding solutions to these relaxed problems converges to the global minimum of the objective function (cf. [**3**]).

(2) *Dynamical Systems Based Optimization (DSO).* A dynamical system is constructed, using a number of sampled values of the objective function to introduce "forces". The evolution of such a system yields a descent trajectory converging to lower values of the objective function. The algorithm continues sampling the domain until it converges to a stationary point (cf. [**49**]).

Our computational results given below for the minimization of (2.26) were obtained by using the open software library `GANSO` (cf. [**26**]), where both the ECAM and DSO methods are implemented.

The optimal trap pattern when N is small, consisting of N traps on one inner sphere, is found to switch to an optimal pattern with $N-1$ traps on an inner sphere and one at the origin as N is increased. We compare the minimal values of the discrete energy $\mathcal{H}_{\text{ball}}$ in (2.26) for the case (a) when all traps are forced to lie on one sphere ($\mathcal{H}_{\text{ball}}^{(a)}$),



(a) $N = 8$ (b) $N = 15$ (c) $N = 16$

FIGURE 1. Numerically computed optimal spatial arrangements of traps inside a unit sphere. For $N = 8$ and $N = 15$ all traps are on an interior sphere. For $N = 16$ there is one trap at the origin, while 15 traps are on an interior sphere.

and in the case (b) when one trap remains at the origin ($r_1 = 0$), while the remaining traps lie on one inner sphere ($\mathcal{H}_{\text{ball}}^{(b)}$). These optimal energy values and the corresponding inner sphere radii, computed with the DSO method, are given in Table 2. For each N with $2 \leq N \leq 15$, our results show that the optimal configuration has N traps located *on a single inner sphere* within the unit sphere. The case $N = 16$ is the smallest value of N that deviates from this rule. In particular, for $16 \leq N \leq 20$, there is one trap located at the origin ($r_1 = 0$), while the remaining $N-1$ traps are located on one interior sphere so that $r_2 =, \ldots, = r_N$.

We remark that the numerically computed minima of the energy function $\mathcal{H}_{\text{ball}}$ in (2.26) were computed directly using the ECAM and DSO methods, and the results obtained were found to coincide with the results shown in Table 2 computed from the restricted optimization problem associated with $\mathcal{H}_{\text{ball}}^{(a)}$ for $2 \leq N \leq 15$ and with $\mathcal{H}_{\text{ball}}^{(b)}$ for $N = 16, 17, 18$. In Fig. 1 we show the numerically computed optimal spatial arrangements of traps for $N = 8, 15, 16$. We also remark that the numerical optimization problem becomes increasingly difficult to solve as N increases, due to the occurrence of many local minima.

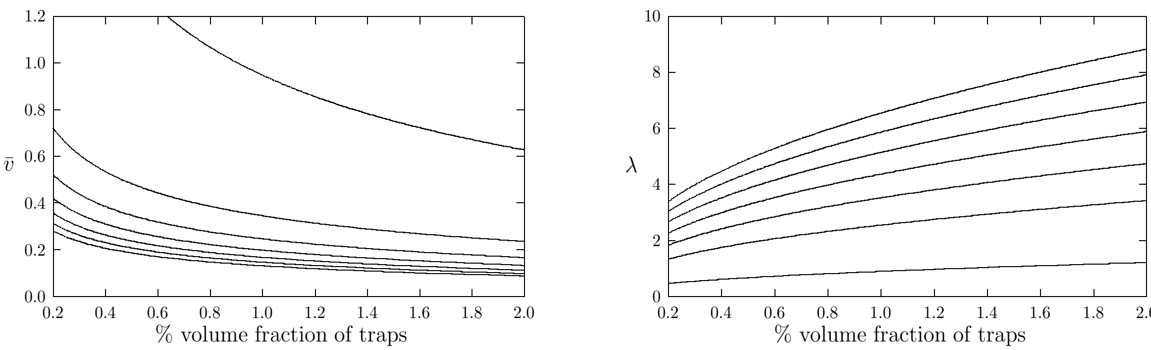
For the special case of N traps with a common capacitance $C = C_j$ for $j = 1, \ldots, N$ inside the unit sphere Ω, then $\bar{v}$ in (2.24) becomes

$$\bar{v} \sim \frac{|\Omega|}{D}\left[\frac{1}{4\pi\varepsilon N C} + \frac{1}{N^2} p(x_1, \ldots, x_N)\right], \qquad p(x_1, \ldots, x_N) = \sum_{i=1}^{N}\sum_{j=1}^{N} \mathcal{G}_{ij} = \frac{\mathcal{H}_{\text{ball}}}{4\pi} - \frac{7N^2}{10\pi}, \tag{2.27}$$

where $\mathcal{H}_{\text{ball}}$ is the discrete energy defined in (2.26). Next, we use (2.27) to illustrate the effect on $\bar{v}$ of trap clustering. For $N = 20$ optimally placed spherical traps of a common radius ε, we set $C = 1$ and use the last entry for $\mathcal{H}_{\text{ball}}$ in Table 2 for $N = 20$ to evaluate p in (2.27). In contrast, suppose that there are $N = 10$ clusters of two touching spheres of a common radius ε inside the unit sphere. Assume that the clusters are optimally located within the unit sphere. For this arrangement, we set $N = 10$ in (2.27), and use the capacitance $C = 2\log 2$ of two touching spheres, together with optimal value for $\mathcal{H}_{\text{ball}}$ given in Table 2 for $N = 10$. In this way, we obtain

$$\bar{v} \sim \frac{|\Omega|}{D}\left(\frac{1}{80\pi\varepsilon} - 0.01871\right), \quad (\text{no trap clustering}); \qquad \bar{v} \sim \frac{|\Omega|}{D}\left(\frac{1}{80\pi\varepsilon\log 2} - 0.02915\right), \quad (\text{trap clustering}). \tag{2.28}$$

Therefore, to leading order, this case of trap clustering increases the average MFPT by a factor of $1/\log 2$.



(a) $\bar{v}$ versus $100f$ (b) λ versus $100f$

FIGURE 2. The average MFPT $\bar{v}$ in (2.24) with $D = 1$ and the principal eigenvalue λ of (2.22 d) versus the percentage trap volume fraction $100f = 100\varepsilon^3 N$ for the optimal arrangement of N identical traps of a common radius ε in the unit sphere. Left figure: $\bar{v}$ versus $100f$ for $N = 1, 5, 8, 11, 14, 17, 20$ (top to bottom curves). Right figure: λ versus $100f$ for $N = 1, 5, 8, 11, 14, 17, 20$ (bottom to top curves).

Principal Result 2.2 can be used to show the influence of the number N of distinct subregions comprising the trap set. In this way, we study the effect of fragmentation of the trap set. We consider N spherical traps of a common radius ε inside the unit sphere. We denote the percentage trap volume fraction by $100f$, where $f = 4\pi\varepsilon^3 N/(3|\Omega|) = \varepsilon^3 N$. In Fig. 2(a) we plot $\bar{v}$, given in (2.27) with $C = 1$, versus the trap volume percentage fraction $100f$ corresponding to the optimal arrangement of $N = 5, 8, 11, 14, 17, 20$ traps, as computed from the global optimization routine discussed above (see Table 2). In this figure we also plot $\bar{v}$ for a single large trap with the same trap volume fraction. We conclude that even when f is small, the effect of fragmentation of the trap set is rather significant. In Fig. 2(b) we plot the corresponding principal eigenvalue λ of (2.22 d) versus the percentage trap volume fraction.

At this stage, we list a few open problems:

(1) Provide reliable computations of the global minimum of the discrete energy $\mathcal{H}_{ball}$ for N large and to determine a scaling law for it that is valid as $N \to \infty$. This scaling law would yield a scaling law for the average MFPT $\bar{v}$.

(2) Does the optimal arrangement of traps for large N exhibit some underlying hexahedron-type symmetry. Can the limiting eigenvalue asymptotics be predicted by the dilute fraction limit of homogenization theory?

(3) Calculate the modified Green's function and its regular part numerically for other 3-D domains to determine the eigenvalue asymptotics as well as a scaling law for the optimal average MFPT. How can one reliably compute the Neumann Green's function in (2.14) for an arbitrary domain given that one must impose the constraint $\int_\Omega G\, dx = 0$.

2.4 Splitting Probabilities

Next, we use the method of matched asymptotic expansions to calculate the splitting probabilities of [**18**]. The splitting probability $u(x)$ is defined as the probability of reaching a specific target trap Ω_{ε_1} from the initial source point $x \in \Omega \backslash \Omega_a$, before reaching any of the other surrounding traps Ω_{ε_j} for $j = 2, \ldots, N$. Then, it is well-known that u satisfies (cf. [**18**])

$$\Delta u = 0 \,, \quad x \in \Omega \backslash \Omega_a \equiv \cup_{j=1}^{N} \Omega_{\varepsilon_j} \,; \qquad \partial_n u = 0 \,, \quad x \in \partial \Omega \,, \tag{2.29 a}$$

$$u = 1 \,, \quad x \in \partial \Omega_{\varepsilon_1} \,; \qquad u = 0 \,, \quad x \in \cup_{j=2}^{N} \partial \Omega_{\varepsilon_j} \,. \tag{2.29 b}$$

By developing a two-term matched asymptotic expansion the following result can be obtained:

<u>**Principal Result 2.3:**</u> *In the limit $\varepsilon \to 0$ of small trap radius, the splitting probability u, satisfying (2.29), is given asymptotically in the outer region $|x - x_j| \gg \mathcal{O}(\varepsilon)$ for $j = 1, \ldots, N$ by*

$$u \sim \frac{C_1}{N\bar{C}} + 4\pi\varepsilon C_1 \left[G(x; x_1) - \frac{1}{N\bar{C}} \sum_{j=1}^{N} C_j G(x; x_j) \right] + \varepsilon \chi_1 + \mathcal{O}(\varepsilon^2) \,, \tag{2.30 a}$$

where χ_1 is given by

$$\chi_1 = -\frac{4\pi C_1}{N\bar{C}} \left[(\mathcal{G}c)_1 - \frac{1}{N\bar{C}} c^T \mathcal{G} c \right] \,. \tag{2.30 b}$$

Here $\mathcal{G}$ is the Green's matrix of (2.23), $c = (C_1, \ldots, C_N)^T$, and $(\mathcal{G}c)_1$ is the first component of $\mathcal{G}c$. The averaged splitting probability $\bar{u} \equiv |\Omega|^{-1} \int_\Omega u \, dx$, which assumes a uniform distribution of starting points $x \in \Omega$, is

$$\bar{u} \sim \frac{C_1}{N\bar{C}} + \varepsilon \chi_1 + \mathcal{O}(\varepsilon^2) \,. \tag{2.30 c}$$

<u>**Problem 2.2:**</u> *Derive Principal Result 2.3 by adapting the methodology of the simple model problem of §2.2.*

The solution to this problem is given in the Appendix A..

From (2.30 a) we observe that $u \sim C_1/(N\bar{C})$, so that there is no leading-order effect on the splitting probability u of either the location of the source, the target, or the surrounding traps. If $C_j = 1$ for $j = 1, \ldots, N$, then $u \sim 1/N$. Therefore, for this equal-capacitance case, then to leading-order in ε it is equally likely to reach any one of the N possible traps. If the target at x_1 has a larger capacitance C_1 than those of the other traps at x_j for $j = 2, \ldots, N$, then the leading order theory predicts that $u > 1/N$. The formulae for the capacitances in Table 1 can be used to calculate the leading order term for u for different shapes of either the target or surrounding traps. Further implications of this result are given in §3 of [**16**].

3 Strong Localized Perturbations in 2-D Domains

In this section we extend the analysis of §2 to treat some related steady-state elliptic problems in a two-dimensional domain with multiple inclusions.

3.1 Some Fundamentals: Leading-Order Eigenvalue Asymptotics

We first recall a basic result from potential theory. Suppose that $\Delta u - k^2 u = \delta(x - x_0)$ for $x \in \Omega \in \mathbb{R}^2$. Then, the singularity has the form

$$u \sim \frac{1}{2\pi} \log|x - x_0| \,, \qquad \text{as} \quad x \to x_0 \,.$$

The derivation of this is simple, and proceeds as in the derivation of the corresponding 3-D result in §3.1.

To illustrate the asymptotic approach and scalings needed in the 2-D case, we consider the following simple eigenvalue problem posed in a domain with a small hole:

$$\begin{cases} \Delta u + \lambda u = 0 & \text{for } x \in \Omega \backslash \Omega_\epsilon \\ u = 0 & \text{for } x \in \partial\Omega \\ u = 0 & \text{for } x \in \partial\Omega_\varepsilon \\ \int_{\Omega\backslash\Omega_\epsilon} u^2 \, dx = 1 \,. \end{cases} \tag{3.1}$$

Here Ω_ϵ is a small hole of "radius" $\mathcal{O}(\varepsilon)$, for which $\Omega_\epsilon \to \{x_0\}$ as $\epsilon \to 0$, where x_0 is an interior point of Ω. Let μ_0, ϕ_0 be the principal first eigenpair of the unperturbed problem, so that

$$\begin{cases} \Delta\phi_0 + \lambda\phi_0 = 0 & \text{for } x \in \Omega \\ \phi_0 = 0 & \text{for } x \in \partial\Omega \\ \int_\Omega \phi_0^2 \, dx = 1 \,. \end{cases} \tag{3.2}$$

Now we will expand the eigenvalue of (3.1) that is close to μ_0 as $\lambda \sim \mu_0 + \nu(\epsilon)\lambda_1 + \cdots$, with $\nu(\epsilon) \to 0$ as $\epsilon \to 0$. Here $\nu(\varepsilon)$ is an unknown gauge function to be determined. In the outer region away from the hole, we expand $u = \phi_0 + \nu u_1 + \cdots$. Upon substituting these expansions into (3.1) we obtain

$$\begin{cases} \Delta u_1 + \mu_0 u_1 = -\lambda_1 \phi_0 & \text{for } x \in \Omega\backslash\{x_0\} \\ u_1 = 0 & \text{for } x \in \partial\Omega \\ \int_\Omega u_1 \phi_0 \, dx = 0 \,. \end{cases} \tag{3.3}$$

In addition, u_1 is to satisfy some singularity condition as $x \to x_0$ that will be determined after constructing the inner expansion and then matching the inner and outer expansions.

In the inner region near the hole, we let $y = \varepsilon^{-1}(x - x_0)$, and we expand $u = \nu(\epsilon) v_0(y) + \cdots$, where $\Delta_y v_0 = 0$. We want $v_0(y) \sim A_0 \log|y|$, as $|y| \to \infty$, and so we write $v_0(y) = A_0 v_c(y)$, where $v_c(y)$ satisfies the canonical inner problem

$$\begin{cases} \Delta_y v_c = 0 & \text{for } y \notin \Omega_0 \\ v_c = 0 & \text{for } y \in \partial\Omega_0 \\ v_c \sim \log|y| & \text{as } |y| \to \infty \,. \end{cases} \tag{3.4 a}$$

The problem (3.4 a) has a unique solution for $v_c(y)$, with the more refined far-field behavior

$$v_c(y) \sim \log|y| - \log d + \mathcal{O}(|y|^{-1}) \,, \quad \text{as} \quad |y| \to \infty \,. \tag{3.4 b}$$

Here d is a constant determined by the solution, and is called the "logarithmic capacitance" of Ω_0.

Notice that, in contrast to the 3-D case, we require that $u \ll \mathcal{O}(1)$ in the inner region. This key point results from

[htbp]

Table 3. The logarithmic capacitance d for some cross-sectional shapes of $\Omega_0 = \varepsilon^{-1}\Omega_\varepsilon$.

Shape of $\Omega_0 \equiv \varepsilon^{-1}\Omega_\varepsilon$	Logarithmic Capacitance d
circle, radius a	$d = a$
ellipse, semi-axes a, b	$d = \frac{a+b}{2}$
equilateral triangle, side h	$d = \frac{\sqrt{3}\,\Gamma\left(\frac{1}{3}\right)^3 h}{8\pi^2} \approx 0.422h$
isosceles right triangle, short side h	$d = \frac{3^{3/4}\Gamma\left(\frac{1}{4}\right)^2 h}{2^{7/2}\pi^{3/2}} \approx 0.476h$
square, side h	$d = \frac{\Gamma\left(\frac{1}{4}\right)^2 h}{4\pi^{3/2}} \approx 0.5902h$

the simple fact that for a prescribed value $C \neq 0$ there is no solution w to the following problem:

$$\Delta_y w = 0\,, \quad y \notin \Omega_0\,,$$
$$w = 0\,, \quad y \in \partial\Omega_0\,; \qquad w \sim C\,, \quad \text{as } |y| \to \infty\,.$$

Therefore, we cannot simply impose in the inner region that $v \sim w + o(1)$ with $w \to \phi_0(x_0)$ as $|y| \to \infty$.

The logarithmic capacitance d depends on the shape of Ω_0 and not its orientation within the domain. A table of numerical values for d for different shapes of Ω_0 are given in [**57**], and some of these are reproduced in Table 3. A boundary integral method to compute d for arbitrarily-shaped domains Ω_1 is described and implemented in [**22**].

Next, we write inner expansion in terms of outer variables as

$$u \sim \nu(\epsilon) A_0 [\log|y| - \log d] \sim \nu(\epsilon) A_0 [-\log(\epsilon d) + \log|x - x_0|]\,,$$

so that the matching condition becomes

$$\phi_0(x_0) + \cdots + \nu(\epsilon) u_1 \sim (-\log(\epsilon d))\, A_0 \nu(\epsilon) + A_0 \nu(\epsilon) \log|x - x_0| + \cdots\,.$$

Therefore, we must take $\nu(\epsilon) = \frac{-1}{\log(\epsilon d)}$ and choose $A_0 = \phi_0(x_0)$. In addition, the matching condition gives the singularity condition $u_1(x) \to A_0 \log|x - x_0| = \phi_0(x_0) \log|x - x_0|$ as $x \to x_0$. Therefore, (3.3) becomes

$$\begin{cases} \Delta u_1 + \mu_0 u_1 = -\lambda_1 \phi_0 & \text{for } x \in \Omega \backslash \{x_0\} \\ u_1 = 0 & \text{for } x \in \partial\Omega \\ u_1 \sim \phi_0(x_0) \log|x - x_0| & \text{as } x \to x_0 \\ \int_\Omega u_1 \phi_0 \, dx = 0\,. \end{cases}$$

This problem is equivalent to

$$\begin{cases} Lu_1 := \Delta u_1 + \mu_0 u_1 = -\lambda_1 \phi_0 + 2\pi \phi_0(x_0) \delta(x - x_0) & \text{for } x \in \Omega \backslash \{x_0\} \\ u_1 = 0 & \text{for } x \in \partial\Omega \\ u_1 \sim \phi_0(x_0) \log|x - x_0| & \text{as } x \to x_0 \\ \int_\Omega u_1 \phi_0 \, dx = 0\,. \end{cases}$$

We then use Green's second identity

$$\int_\Omega (\phi_0 \partial_n u_1 - u_1 \partial_n \phi_0)\, dS = \int_\Omega (\phi_0 L u_1 - u_1 L \phi_0)\, dx\,,$$

with $\phi_0 = u_1 = 0$ on $\partial\Omega$ and $L\phi_0 = 0$. In this way, we get $\int_\Omega \phi_0 L u_1 \, dx = 0$, which can be written as

$$\int_\Omega \phi_0 \left(-\lambda_1 \phi_0 + 2\pi \phi_0(x_0)\delta(x - x_0)\right) \, dx = 0 \, .$$

This specifies λ_1 as

$$\lambda_1 = \frac{2\pi [\phi_0(x_0)]^2}{\int_\Omega \phi_0^2 \, dx} \, .$$

Therefore, we obtain a two-term expansion for the perturbation of the fundamental eigenvalue given by

$$\lambda \sim \mu_0 + \frac{2\pi \nu [\phi_0(x_0)]^2}{\int_\Omega \phi_0^2 \, dx} + \cdots \, , \qquad \nu = -\frac{1}{\log(\epsilon d)} \, . \tag{3.6}$$

Remarks:

(1) Further terms in the expansion have the form

$$\lambda \sim \mu_0 + A_1 \nu + A_2 \nu^2 + A_3 \nu^3 + \cdots \, ,$$

which is an infinite-logarithmic expansion in powers of ν. Since $(\log(\epsilon d))^{-1}$ decreases only very slowly in ε, it would be preferable to find a method to "sum" the series. Such a method is developed and implemented in later subsections. In particular, is the series convergent when ε is small, or only asymptotic? Our results below indicate that the series is in fact convergent for ε sufficiently small.

(2) If $u = 0$ on $\partial\Omega$ is replaced by $\partial_n u = 0$ on $\partial\Omega$, then $\mu_0 = 0$ and $\phi_0 = \frac{1}{\sqrt{|\Omega|}}$ so that $\int_\Omega \phi_0^2 dx = 1$. This yields the leading-order result

$$\lambda \sim \frac{2\pi\nu}{|\Omega|} \, , \quad \text{as} \quad \epsilon \to 0 \, .$$

Therefore, the leading-order asymptotics is independent of the location of the hole. Further terms in the expansion of the eigenvalue must be obtained to determine the effect of the location of the hole. This is done in §3.3 – §3.5 for various problems where the leading-order asymptotics gives no information.

For an annular domain, we now confirm our two-term asymptotic result by comparing it with the result obtained by expanding the exact eigenvalue relation for small ε. The eigenvalue problem in an annular domain is

$$\begin{cases} \Delta u + \lambda u = 0 & \text{in } \epsilon < r < 1 \\ u = 0 & \text{on } r = 1 \\ u = 0 & \text{on } r = \epsilon \, . \end{cases}$$

The unperturbed solution is $\phi_0 = J_0(\sqrt{\mu_0} r)$ where $J_0(\sqrt{\mu_0}) = 0$ and $\sqrt{\mu_0} = \tau_0$, with z_0 is the first zero of $J_0(z)$.

Using the perturbation formula we have $v_c(y) = \log |y|$, since $\Delta_y v_c = 0$, $v_c = 0$ on $|y| = 1$, so that $d = 1$. Then, $x_0 = 0$ and $\phi_0(x_0) = J_0(0) = 1$. Therefore, from (3.6), we obtain

$$\lambda \sim \mu_0 + \frac{2\pi\nu}{\int_\Omega \phi_0^2(x) \, dx} \sim \mu_0 + \frac{2\pi\nu}{2\pi \int_0^1 r J_0^2(\sqrt{\mu_0} r) \, dr} \, .$$

We recall the integral identity $\int_0^1 r J_0^2(\sqrt{\mu_0} r) \, dr = \frac{1}{2}(J_0'(\sqrt{\mu_0}))^2$, when $J_0(\sqrt{\mu_0}) = 0$, so that the expression above becomes

$$\lambda \sim \mu_0 + \left(-\frac{1}{\log(\epsilon)} \right) \left(\frac{2}{\left[J_0'(\sqrt{\mu_0}) \right]^2} \right) + \cdots . \tag{3.7}$$

Now we compare (3.7) with the exact solution. In the class of radially symmetric eigenfunctions, we obtain

$$u = J_0(\sqrt{\lambda} r) - \frac{J_0(\sqrt{\lambda})}{Y_0(\sqrt{\lambda})} Y_0(\sqrt{\lambda} r) .$$

Setting $u(\varepsilon) = 0$ gives the eigenvalue relation as

$$J_0(\sqrt{\lambda}) = \frac{J_0(\sqrt{\lambda}\epsilon)}{Y_0(\sqrt{\lambda}\epsilon)} Y_0(\sqrt{\lambda}) . \tag{3.8}$$

To solve this eigenvalue relation for $\varepsilon \ll 1$, we first recall that

$$J_0(z) \sim 1 + \mathcal{O}(z^2) \qquad Y_0(z) \sim \frac{2}{\pi} [\log(z) - \log 2 + \gamma] + \cdots , \qquad \text{as} \quad z \to 0 ,$$

where γ is Euler's constant. Therefore, with $z = \sqrt{\lambda}$ we obtain for $\varepsilon \ll 1$ that (3.8) becomes

$$J_0(z) \sim Y_0(z) \frac{\pi}{2} [\log(\epsilon z) - \log 2 + \gamma]^{-1} .$$

To find the root of this expression we expand

$$z = z_0 + \left(\frac{-1}{\log \varepsilon} \right) z_1 + \cdots ,$$

Here $z_0 = \sqrt{\lambda_0}$ is the first root of $J_0(z_0) = 0$, so that $z_0 = \sqrt{\mu_0}$. Then, we use Taylor series to obtain

$$J_0(z_0) + \left(\frac{-1}{\log \varepsilon} \right) J_0'(z_0) z_1 + \ldots \sim \frac{\pi Y_0(z_0)}{2 \log \epsilon} + \cdots .$$

This yields that $z_1 = -\frac{\pi}{2} \frac{Y_0(z_0)}{J_0'(z_0)}$. Now we write $\sqrt{\lambda} = z = z_0 + \left(-\frac{1}{\log \epsilon} \right) z_1 + \cdots$. Hence, we get $\lambda \sim z_0^2 + \left(-\frac{1}{\log \epsilon} \right) 2 z_0 z_1 + \ldots$, which yields $\lambda \sim \mu_0 + \left(-\frac{1}{\log \epsilon} \right) 2\sqrt{\mu_0} z_1$. In summary, we obtain that

$$\lambda \sim \mu_0 + \left(-\frac{1}{\log \epsilon} \right) \lambda_1 + \cdots , \qquad \lambda_1 = 2\sqrt{\mu_0} z_1 = 2\sqrt{\mu_0} \left(-\frac{\pi}{2} \frac{Y_0(\sqrt{\mu_0})}{J_0'(\sqrt{\mu_0})} \right) = -\pi\sqrt{\mu_0} \frac{Y_0(\sqrt{\mu_0})}{J_0'(\sqrt{\mu_0})} . \tag{3.9}$$

To write this result in a form to compare with the result obtained above from the asymptotic theory, we need an identity that is based on the Wronskian relation

$$\left(\frac{\mathrm{d}}{\mathrm{d}r} J_0(\sqrt{\lambda} r) \right) Y_0(\sqrt{\lambda} r) - \left(\frac{\mathrm{d}}{\mathrm{d}r} Y_0(\sqrt{\lambda} r) \right) J_0(\sqrt{\lambda} r) = -\frac{2}{\pi r} .$$

Now evaluating this identity at $r = 1$, and setting $\lambda = \mu_0$ where $J_0(\sqrt{\mu_0}) = 0$, we get

$$Y_0(\sqrt{\mu_0}) = \frac{2}{\pi \sqrt{\mu_0} J_0'(\sqrt{\mu_0})} .$$

Substituting this into the result of (3.9) we obtain

$$\lambda_1 = -\pi\sqrt{\mu_0} \left(\frac{Y_0(\sqrt{\mu_0})}{J_0'(\sqrt{\mu_0})} \right) = \frac{2}{(J_0'(\sqrt{\mu_0}))^2} ,$$

which gives the two-term expansion

$$\lambda \sim \mu_0 + \left(-\frac{1}{\log \epsilon} \right) \frac{2}{(J_0'(\sqrt{\mu_0}))^2} + \cdots ,$$

in agreement with the asymptotic result given in (3.7).

In the next section we consider a simple problem to illustrate the methodology used to sum infinite logarithmic expansions for singularly perturbed PDE problems in 2-D domains with holes.

3.2 Summing the Infinite Logarithmic Expansion: A Simple Model Problem

We first consider a simple problem to illustrate some main ideas for treating elliptic PDE problems with infinite logarithmic expansions. Consider a two-dimensional bounded domain Ω with a small trap Ω_ε of radius $\mathcal{O}(\varepsilon)$ centered at some $x_0 \in \Omega$. Then, the expected time $w(x)$ for a Brownian particle to be captured given that it starts from $x \in \Omega\backslash\Omega_\varepsilon$ satisfies Poisson's equation

$$\triangle w = -\beta \equiv -1/D\,, \quad x \in \Omega\backslash\Omega_\varepsilon\,, \tag{3.10 a}$$

$$w = 0\,, \quad x \in \partial\Omega\,, \tag{3.10 b}$$

$$w = 0\,, \quad x \in \partial\Omega_\varepsilon\,. \tag{3.10 c}$$

where D is the constant diffusivity. We assume that Ω_ε has radius $\mathcal{O}(\varepsilon)$ and that $\Omega_\varepsilon \to x_0$ uniformly as $\varepsilon \to 0$, where $x_0 \in \Omega$. We denote the scaled subdomain that results from an $\mathcal{O}(\varepsilon^{-1})$ magnification of the length scale of Ω_ε by $\Omega_1 \equiv \varepsilon^{-1}\Omega_\varepsilon$. In this model problem the outer boundary on $\partial\Omega$ is also absorbing.

The asymptotic solution to (3.10) is constructed in two different regions: an outer region defined at an $\mathcal{O}(1)$ distance from the localized trap, and an inner region defined in an $\mathcal{O}(\varepsilon)$ neighborhood of the trap Ω_ε. The analysis below will show how to calculate the sum of all the logarithmic terms for w in in the limit $\varepsilon \to 0$ of small core radius.

In the outer region we expand the solution to (3.10) as

$$w(x;\varepsilon) = W_0(x;\nu) + \sigma(\varepsilon)W_1(x;\nu) + \cdots\,. \tag{3.11}$$

Here $\nu = \mathcal{O}(1/\log\varepsilon)$ is a gauge function to be chosen, and we assume that $\sigma \ll \nu^k$ for any $k > 0$ as $\varepsilon \to 0$. Thus, W_0 contains all of the logarithmic terms in the expansion. Substituting (3.11) into (3.10 a) and (3.10 b), and letting $\Omega_\varepsilon \to x_0$ as $\varepsilon \to 0$, we get that W_0 satisfies

$$\triangle W_0 = -\beta\,, \quad x \in \Omega\backslash\{x_0\}\,, \tag{3.12 a}$$

$$W_0 = 0\,, \quad x \in \partial\Omega\,, \tag{3.12 b}$$

$$W_0 \quad \text{is singular as} \quad x \to x_0\,. \tag{3.12 c}$$

The matching of the outer and inner expansions will determine a singularity behavior for W_0 as $x \to x_0$.

In the inner region near Ω_ε we introduce the inner variables

$$y = \varepsilon^{-1}(x - x_0)\,, \qquad v(y;\varepsilon) = W(x_0 + \varepsilon y;\varepsilon)\,. \tag{3.13}$$

If we naively assume that $v = \mathcal{O}(1)$ in the inner region, we obtain the leading-order problem for v that $\triangle_y v = 0$ outside Ω_1, with $v = 0$ on $\partial\Omega_1$ and $v \to W_0(x_0)$ as $|y| \to \infty$, where $\triangle_y$ denotes the Laplacian in the y variable. This far-field condition as $|y| \to \infty$ is obtained by matching v to the outer solution. However, in two-dimensions there is no solution to this problem since the Green's function for the Laplacian grows logarithmically at infinity. To overcome this difficulty, we require that $v = \mathcal{O}(\nu)$ in the inner region and we allow v to be logarithmically unbounded as $|y| \to \infty$. Therefore, we expand v as

$$v(y;\varepsilon) = V_0(y;\nu) + \mu_0(\varepsilon)V_1(y) + \cdots \,, \tag{3.14 a}$$

where we write V_0 in the form

$$V_0(y;\nu) = \nu\gamma v_c(y) \,. \tag{3.14 b}$$

Here $\gamma = \gamma(\nu)$ is a constant to be determined with $\gamma = \mathcal{O}(1)$ as $\nu \to 0$, and we assume that $\mu_0 \ll \nu^k$ for any $k > 0$ as $\varepsilon \to 0$. Substituting (3.13) and (3.14) into (3.10 *a*) and (3.10 *c*), and allowing $v_c(y)$ to grow logarithmically at infinity, we obtain that $v_c(y)$ satisfies

$$\triangle_y v_c = 0 \,, \quad y \notin \Omega_1 \,; \qquad v_c = 0 \,, \quad y \in \partial\Omega_1 \,, \tag{3.15 a}$$

$$v_c \sim \log|y| \,, \quad \text{as} \quad |y| \to \infty \,. \tag{3.15 b}$$

The unique solution to (3.15) has the following far-field asymptotic behavior:

$$v_c(y) \sim \log|y| - \log d + \frac{p \cdot y}{|y|^2} + \cdots \,, \quad \text{as} \quad |y| \to \infty \,. \tag{3.15 c}$$

The constant $d > 0$ is the logarithmic capacitance of Ω_1, while the vector p is called the dipole vector.

The leading-order matching condition between the inner and outer solutions will determine the constant γ in (3.14 *b*). Upon writing (3.15 *c*) in outer variables and substituting into (3.14 *b*), we get the far-field behavior

$$v(y;\varepsilon) \sim \gamma\nu \left[\log|x - x_0| - \log(\varepsilon d)\right] + \cdots \,, \quad \text{as} \quad |y| \to \infty \,. \tag{3.16}$$

Choosing

$$\nu(\varepsilon) = -1/\log(\varepsilon d) \,, \tag{3.17}$$

and matching (3.16) to the outer expansion (3.11) for W, we obtain the singularity condition for W_0,

$$W_0 = \gamma + \gamma\nu \log|x - x_0| + o(1) \,, \quad \text{as} \quad x \to x_0 \,. \tag{3.18}$$

The singularity behavior in (3.18) specifies both the regular and singular part of a Coulomb singularity. As such, it provides one constraint for the determination of γ. More specifically, the solution to (3.12) together with (3.18) must determine γ, since for a singularity condition of the form $W_0 \sim S \log|x - x_0| + R$ for an elliptic equation, the constant R is not arbitrary but is determined as a function of S, x_0, and Ω.

The solution for W_0 is decomposed as

$$W_0(x;\nu) = W_{0H}(x) - 2\pi\gamma\nu G_d(x;x_0) \,. \tag{3.19}$$

Here $W_{0H}(x)$ is the smooth function satisfying the unperturbed problem

$$\triangle W_{0H} = -\beta \,, \quad x \in \Omega \,; \qquad W_{0H} = 0 \,, \quad x \in \partial\Omega \,. \tag{3.20}$$

In (3.19), $G_d(x;x_0)$ is the Dirichlet Green's function satisfying

$$\triangle G_d = -\delta(x-x_0)\,, \quad x\in\Omega\,; \qquad G_d = 0\,, \quad x\in\partial\Omega\,, \tag{3.21 a}$$

$$G_d(x;x_0) = -\frac{1}{2\pi}\log|x-x_0| + R_d(x_0;x_0) + o(1)\,, \quad \text{as} \quad x\to x_0\,. \tag{3.21 b}$$

Here $R_{d00}\equiv R_d(x_0;x_0)$ is the regular part of the Dirichlet Green's function $G_d(x;x_0)$ at $x=x_0$. This regular part is also known as either the self-interaction term or the Robin constant (cf. [**2**]).

Upon substituting (3.21 b) into (3.19) and letting $x\to x_0$, we compare the resulting expression with (3.18) to obtain that γ is given by

$$\gamma = \frac{W_{0H}(x_0)}{1+2\pi\nu R_{d00}}\,. \tag{3.22}$$

Therefore, for this problem, γ is determined as the sum of a geometric series in ν. The range of validity of (3.22) is limited to values of ε for which $2\pi\nu|R_{d00}|<1$. This yields,

$$0<\varepsilon<\varepsilon_c\,, \qquad \varepsilon_c \equiv \frac{1}{d}\exp\left[2\pi R_{d00}\right]\,. \tag{3.23}$$

We summarize our result as follows:

<u>Principal Result 3.1:</u> *For $\varepsilon\ll 1$, the outer expansion for (3.10) is*

$$w\sim W_0(x;\nu) = W_{0H}(x) - \frac{2\pi\nu W_{0H}(x_0)}{1+2\pi\nu R_{d00}}G_d(x;x_0)\,, \quad \text{for} \quad |x-x_0|=\mathcal{O}(1)\,, \tag{3.24 a}$$

and the inner expansion with $y=\varepsilon^{-1}(x-x_0)$ is

$$w\sim V_0(y;\nu) = \frac{\nu W_{0H}(x_0)}{1+2\pi\nu R_{d00}}v_c(y)\,, \quad \text{for} \quad |x-x_0|=\mathcal{O}(\varepsilon)\,. \tag{3.24 b}$$

Here $\nu=-1/\log(\varepsilon d)$, d is defined in (3.15 c), $v_c(y)$ satisfies (3.15), and W_{0H} satisfies the unperturbed problem (3.20). Also $G_d(x;x_0)$ and $R_{d00}\equiv R_d(x_0;x_0)$ are the Dirichlet Green's function and its regular part satisfying (3.21).

This formulation is referred to as a hybrid asymptotic-numerical method since it uses the asymptotic analysis as a means of reducing the original problem (3.10) with a hole to the simpler asymptotically related problem (3.12) with singularity behavior (3.18). This related problem does not have a boundary layer structure and so is easy to solve numerically. The numerics required for the hybrid problem involve the computation of the unperturbed solution W_{0H} and the Dirichlet Green's function $G_d(x;x_0)$. In terms of G_d we then identify its regular part $R_d(x_0;x_0)$ at the singular point. From the solution to the canonical inner problem (3.15) we then compute the logarithmic capacitance, d. The result (3.24 a) then shows that the asymptotic solution only depends on the product of εd and not on ε itself. This feature allows for an asymptotic equivalence between traps of different cross-sectional shape, based on an effective 'radius' of the trap. This equivalence is known as Kaplun's equivalence principle (cf. [**33**], [**40**]).

An advantage of the hybrid method over the traditional method of matched asymptotic expansions is that the hybrid formulation is able to sum the infinite logarithmic series and thereby provide an accurate approximate solution. From another viewpoint, the hybrid problem is much easier to solve numerically than the full singularly perturbed problem (3.10). For the hybrid method a change of the shape of Ω_1 requires us to only re-calculate the constant

d. This simplification does not occur in a full numerical approach. An explicit example comparing the result of the hybrid method with a full numerical solution is given in [**75**].

We now outline how Principal Result 3.1 can be obtained by a direct summation of a conventional infinite-order logarithmic expansion for the outer solution given in the form

$$W \sim W_{0H}(x) + \sum_{j=1}^{\infty} \nu^j W_{0j}(x) + \mu_0(\varepsilon) W_1 + \cdots \,, \tag{3.25}$$

with $\mu_0(\varepsilon) \ll \nu^k$ for any $k > 0$. By formulating a similar series for the inner solution, we will derive a recursive set of problems for the W_{0j} for $j \geq 0$ from the asymptotic matching of the inner and outer solutions. We will then sum this series to re-derive the result in Principal Result 3.1.

In the outer region we expand the solution to (3.10) as in (3.25). In (3.25), $\nu = \mathcal{O}(1/\log \varepsilon)$ is a gauge function to be chosen, while the smooth function W_{0H} satisfies the unperturbed problem (3.20) in the unperturbed domain. By substituting (3.25) into (3.10 a) and (3.10 b), and letting $\Omega_\varepsilon \to x_0$ as $\varepsilon \to 0$, we get that W_{0j} for $j \geq 1$ satisfies

$$\triangle W_{0j} = 0 \,, \quad x \in \Omega \backslash \{x_0\} \,, \tag{3.26 a}$$

$$W_{0j} = 0 \,, \quad x \in \partial\Omega \,, \tag{3.26 b}$$

$$W_{0j} \quad \text{is singular as} \quad x \to x_0 \,. \tag{3.26 c}$$

The matching of the outer and inner expansions will determine a singularity behavior for W_{0j} as $x \to x_0$ for each $j \geq 1$.

In the inner region near Ω_ε we introduce the inner variables

$$y = \varepsilon^{-1}(x - x_0) \,, \qquad v(y;\varepsilon) = W(x_0 + \varepsilon y; \varepsilon) \,. \tag{3.27}$$

We then pose the explicit infinite-order logarithmic inner expansion

$$v(y;\varepsilon) = \sum_{j=0}^{\infty} \gamma_j \nu^{j+1} v_c(y) \,. \tag{3.28}$$

Here γ_j are ε-independent coefficients to be determined. Substituting (3.28) and (3.10 a) and (3.10 c), and allowing $v_c(y)$ to grow logarithmically at infinity, we obtain that $v_c(y)$ satisfies (3.15) with far-field behavior (3.15 c).

Upon using the far-field behavior (3.15 c) in (3.28), and writing the resulting expression in terms of the outer variable $x - x_0 = \varepsilon y$, we obtain that

$$v \sim \gamma_0 + \sum_{j=1}^{\infty} \nu^j \left[\gamma_{j-1} \log|x - x_0| + \gamma_j \right] \,. \tag{3.29}$$

The matching condition between the infinite-order outer expansion (3.25) as $x \to x_0$ and the far-field behavior (3.29) of the inner expansion is that

$$W_{0H}(x_0) + \sum_{j=1}^{\infty} \nu^j W_{0j}(x) \sim \gamma_0 + \sum_{j=1}^{\infty} \nu^j \left[\gamma_{j-1} \log|x - x_0| + \gamma_j \right] \,. \tag{3.30}$$

The leading-order match yields that

$$\gamma_0 = W_{0H}(x_0) \,. \tag{3.31}$$

The higher-order matching condition, from (3.30), shows that the solution W_{0j} to (3.26) must have the singularity behavior

$$W_{0j} \sim \gamma_{j-1} \log|x-x_0| + \gamma_j \,, \quad \text{as} \quad x \to x_0 \,. \tag{3.32}$$

The unknown coefficients γ_j for $j \geq 1$, starting with $\gamma_0 = W_{0H}(x_0)$, are determined recursively from the infinite sequence of problems (3.26) and (3.32) for $j \geq 1$. The explicit solution to (3.26) with $W_{0j} \sim \gamma_{j-1} \log|x-x_0|$ as $x \to x_0$ is given explicitly in terms of $G_d(x;x_0)$ of (3.21) as

$$W_{0j}(x) = -2\pi\gamma_{j-1} G_d(x;x_0) \,. \tag{3.33}$$

Next, we expand (3.33) as $x \to x_0$ and compare it with the required singularity structure (3.32). This yields

$$-2\pi\gamma_{j-1}\left[-\frac{1}{2\pi}\log|x-x_0| + R_{d00}\right] \sim \gamma_{j-1}\log|x-x_0| + \gamma_j \,, \tag{3.34}$$

where $R_{d00} \equiv R_d(x_0;x_0)$. By comparing the non-singular parts of (3.34), we obtain a recursion relation for the γ_j, valid for $j \geq 1$, given by

$$\gamma_j = (-2\pi R_{d00})\,\gamma_{j-1} \,, \qquad \gamma_0 = W_{0H}(x_0) \,, \tag{3.35}$$

which has the explicit solution

$$\gamma_j = \left[-2\pi R_{d00}\right]^j W_{0H}(x_0) \,, \quad j \geq 0 \,. \tag{3.36}$$

Finally, to obtain the outer solution we substitute (3.33) and (3.36) into (3.25) to obtain

$$\begin{aligned} w - W_{0H}(x) &\sim \sum_{j=1}^{\infty} \nu^j \left(-2\pi\gamma_{j-1}\right) G_d(x;x_0) = -2\pi\nu G_d(x;x_0) \sum_{j=0}^{\infty} \nu^j \gamma_j \\ &\sim -2\pi\nu W_{0H}(x_0) G_d(x;x_0) \sum_{j=0}^{\infty} \left[-2\pi\nu R_{d00}\right]^j \\ &\sim -\frac{2\pi\nu W_{0H}(x_0)}{1+2\pi\nu R_{d00}} G_d(x_0;x_0) \,. \end{aligned} \tag{3.37 a}$$

Equation (3.37 a) agrees with equation (3.24 a) of Principal Result 3.1. Similarly, upon substituting (3.36) into the infinite-order inner expansion (3.28), we obtain

$$v(y;\varepsilon) = \nu W_{0H}(x_0) v_c(y) \sum_{j=0}^{\infty} \left[-2\pi R_{d00}\nu\right]^j = \frac{\nu W_{0H}(x_0)}{1+2\pi\nu R_{d00}} v_c(y) \,, \tag{3.38}$$

which recovers equation (3.24 b) of Principal Result 3.1. This derivation strongly suggests that infinite logarithmic expansions are not just asymptotic, but actually do converge when ε is sufficiently small.

At this stage, the reader should attempt the following two problems (with solutions given in Appendix B):

Problem 3.1: *Consider the following problem in an arbitrary two-dimensional domain with N small inclusions:*

$$\triangle u - m(x) u = 0 \,, \qquad x \in \Omega \backslash \cup_{j=1}^{N} \Omega_{\varepsilon_j} \,, \tag{3.39 a}$$

$$u = \alpha_j \,, \qquad x \in \partial\Omega_{\varepsilon_j} \,, \quad j = 1, \ldots, N \,, \tag{3.39 b}$$

$$u = f \,, \qquad x \in \partial\Omega \,. \tag{3.39 c}$$

Here $m(x)$ is an arbitrary smooth function with $m(x) > 0$ in Ω, f is an arbitrary function on $\partial\Omega$, and α_j are *constants. Formulate a linear system in terms of a certain Green's function, that effectively sums the infinite-order logarithmic series in the asymptotic expansion of the solution. Apply your general theory to the unit disk Ω for the case $N = 1$, $m \equiv 1$, $f \equiv 0$, and $\alpha_1 = 1$, when there is an arbitrarily-shaped hole centered at the origin of the unit disk.*

<u>Problem 3.2:</u> *Consider the following problem in the disk $\Omega = \{x \,|\, |x| \leq 2\}$ that contains three small holes:*

$$\triangle u = 0 \,, \qquad x \in \Omega \backslash \cup_{j=1}^{3} \Omega_{\varepsilon_j} \,, \tag{3.40 a}$$

$$u = \alpha_j \,, \qquad x \in \partial\Omega_{\varepsilon_j} \,, \quad j = 1, 2, 3 \,, \tag{3.40 b}$$

$$u = 4\cos(2\theta) \,, \qquad |x| = 2 \,. \tag{3.40 c}$$

Suppose that each of the holes has an elliptical shape with semi-axes ε and 2ε. Apply the theory for summing infinite logarithmic expansions to first derive and then numerically solve a linear system for the source strengths. In your implementation assume that the holes are centered at $x_1 = (1/2, 1/2)$, $x_2 = (1/2, 0)$ and $x_3 = (-1/4, 0)$. The boundary values on the holes are to be taken as $\alpha_1 = 1$, $\alpha_2 = 0$ and $\alpha_3 = 2$.

3.3 The Principal Neumann Eigenvalue in a Planar Domain with Traps

In this section we follow [**38**] and consider an optimization problem for the fundamental eigenvalue of the Laplacian in a planar bounded two-dimensional domain with a reflecting boundary that is perturbed by the presence of K small holes in the interior of the domain. The perturbed eigenvalue problem is

$$\Delta u + \lambda u = 0 \,, \quad x \in \Omega \backslash \Omega_p \,; \quad \int_{\Omega \backslash \Omega_p} u^2 \, dx = 1 \,, \tag{3.41 a}$$

$$\partial_n u = 0 \,, \quad x \in \partial\Omega \,; \quad u = 0 \,, \quad x \in \partial\Omega_p \equiv \cup_{i=1}^{K} \partial\Omega_{\varepsilon_i} \,. \tag{3.41 b}$$

Here Ω is the unperturbed domain, $\Omega_p = \cup_{i=1}^{K} \Omega_{\varepsilon_i}$ is a collection of K small interior holes Ω_{ε_i}, for $i = 1, \ldots, K$, each of 'radius' $\mathcal{O}(\varepsilon)$, and $\partial_n u$ is the outward normal derivative of u on $\partial\Omega$. We assume that the small holes in Ω are non-overlapping and that $\Omega_{\varepsilon_i} \to x_i$ as $\varepsilon \to 0$, for $i = 1, \ldots, K$. A schematic plot of the domain is shown in Fig. 3.

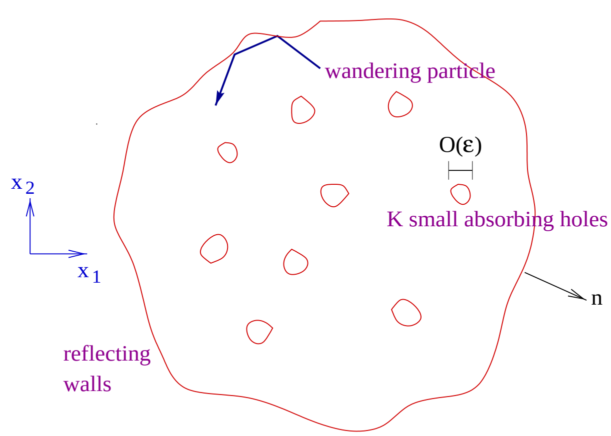


FIGURE 3. A schematic plot of the perturbed domain for the eigenvalue problem (3.41).

We let $\lambda_0(\varepsilon)$ denote the first eigenvalue of (3.41), with corresponding eigenfunction $u(x, \varepsilon)$. Clearly, $\lambda_0(\varepsilon) \to 0$ as

$\varepsilon \to 0$. Our objective is to determine the locations, x_i for $i = 1, \ldots, K$, of the K holes of a given shape that maximize this fundamental eigenvalue. Asymptotic expansions for the fundamental eigenvalue of related eigenvalue problems in perforated multi-dimensional domains, with various boundary conditions on the holes and outer boundary, are given in [**51**], [**77**], [**78**], [**20**], and [**43**] (see also the references therein).

As an application of (3.41), consider the Brownian motion of a particle in a two-dimensional domain Ω, with reflecting walls, that contains K small traps Ω_{ε_i}, for $i = 1, \ldots, K$, each of 'radius' ε, for $i = 1, \ldots, K$. The traps are centered at x_i, for $i = 1, \ldots, K$. If the Brownian particle starts from the point $y \in \Omega \backslash \Omega_p$ at time $t = 0$, then the probability density $v(x, y, t, \varepsilon)$ that the particle is at point x at time t satisfies

$$v_t = \Delta v \,, \quad x \in \Omega \backslash \Omega_p \,; \quad \partial_n v = 0 \,, \quad x \in \partial\Omega \,; \quad v = 0 \,, \quad x \in \partial\Omega_p \,; \quad v = \delta(x - y) \,, \quad t = 0 \,. \tag{3.42}$$

By calculating the solution to (3.42) in terms of an eigenfunction expansion, and by assuming that y is uniformly distributed over $\Omega \backslash \Omega_p$, it is easy to show that the probability $P_0(t, \varepsilon)$ that the Brownian particle is in $\Omega \backslash \Omega_p$ at time t is given by

$$P_0(t, \varepsilon) = e^{-\lambda_0(\varepsilon) t} \left[1 + \mathcal{O}(\nu) \right] \,. \tag{3.43}$$

Therefore, the expected lifetime of the Brownian particle is proportional to $1/\lambda_0(\varepsilon)$. In this context, our optimization problem is equivalent to choosing the locations of K small traps to minimize this expected lifetime.

We first consider (3.41) for the case of one hole. In [**77**] (see also [**78**]) it was shown that as $\varepsilon \to 0$ the first eigenvalue λ_0 of (3.41) has the asymptotic expansion:

$$\lambda_0(\varepsilon) = \lambda_{00} + \nu(\varepsilon)\lambda_{01} + \nu^2(\varepsilon)\lambda_{02} + \cdots \,.$$

Here, $\nu(\varepsilon) = -1/\log(\varepsilon d)$ where d is the logarithmic capacitance of the hole. For the unperturbed problem with $\varepsilon = 0$, we have $\lambda_{00} = 0$. In the $\mathcal{O}(\nu)$ term, λ_{01} is independent of the location of the hole at $x = x_0$ (cf. [**77**]). Therefore, we need the higher-order coefficient λ_{02} in order to determine the location of the hole that maximizes the first eigenvalue, λ_0.

For the case of one hole, an infinite logarithmic expansion for $\lambda_0(\varepsilon)$ has the form

$$\lambda_0(\varepsilon) = \lambda^*(\nu) + \mathcal{O}\left(\frac{\varepsilon}{\log \varepsilon} \right) \,, \qquad \nu \equiv -\frac{1}{\log(\varepsilon d)} \,.$$

To calculate $\lambda^*(\nu)$ we use the hybrid asymptotic-numerical method of [**38**]. Near the hole, we identify an inner (local) region in terms of a local spatial variable $y = \varepsilon^{-1}(x - x_0)$, and where the hole is rescaled so that $\Omega_0 \equiv \varepsilon^{-1}\Omega_\varepsilon$. Denoting the inner (local) solution by $v(y, \varepsilon) = u(x_0 + \varepsilon y, \varepsilon)$, we then expand $v(y, \varepsilon)$ as

$$v(y, \varepsilon) = A \, \nu \, v_c(y) + \cdots \,. \tag{3.44}$$

Here, $A = A(\nu) \sim \mathcal{O}(1)$ as $\varepsilon \to 0$, and $v_c(y)$ is the solution of the canonical inner problem (3.15), re-written here as

$$\Delta_y v_c = 0 \,, \quad y \notin \Omega_0 \,; \quad v_c = 0 \,, \quad y \in \partial\Omega_0 \,, \tag{3.45 a}$$

$$v_c \sim \log|y| - \log d + \frac{p \cdot y}{|y|^2} \,, \quad \text{as} \quad |y| \to \infty \,. \tag{3.45 b}$$

In (3.45 b), the logarithmic capacitance d and the dipole vector $p = (p_1, p_2)$ are determined from the shape of the hole.

We expand the eigenvalue λ_0 and the outer (global) solution as

$$\lambda_0(\varepsilon) = \lambda^*(\nu) + \mu\lambda_1 + \cdots, \qquad u(x,\varepsilon) = u^*(x,\nu) + \mu u_1(x,\nu) + \cdots, \tag{3.46}$$

where $\mu \ll \mathcal{O}(\nu^k)$ for any $k > 0$. Substituting (3.46) into (3.41 a) and the boundary condition (3.41 b) on $\partial\Omega$, we obtain the full problem in a domain punctured by the point x_0,

$$\Delta u^* + \lambda^* u^* = 0, \quad x \in \Omega\backslash\{x_0\}; \quad \int_\Omega (u^*)^2\, dx = 1; \quad \partial_n u^* = 0, \quad x \in \partial\Omega. \tag{3.47}$$

The singularity condition for (3.47) as $x \to x_0$ given below arises from matching u^* to the inner solution. Substituting (3.45 b) into (3.44), and expressing the result in global variables, we obtain

$$v(y,\varepsilon) \sim A\,\nu \log|x - x_0| + A + \varepsilon A\,\nu \frac{p\cdot(x-x_0)}{|x-x_0|^2} + \cdots, \quad \text{as} \quad y \to \infty. \tag{3.48}$$

Here, we have used $\nu \equiv -1/\log(\varepsilon d)$. To match u^* to (3.48), we require that u^* has the singularity behavior

$$u^*(x,\nu) \sim A\,\nu\, \log|x - x_0| + A, \quad \text{as} \quad x \to x_0. \tag{3.49}$$

Comparing the terms in (3.48) and (3.46) at the next order, we see that $\mu = \mathcal{O}(\varepsilon\nu)$.

Next, we determine $u^*(x,\nu)$ and $\lambda^*(\nu)$ satisfying (3.47) and (3.49). To do so, we introduce the Helmholtz Green's function, $G_h(x;x_0,\lambda^*)$, and its regular part, $R_h(x_0;x_0,\lambda^*)$, satisfying

$$\Delta G_h + \lambda^* G_h = -\delta(x - x_0), \quad x \in \Omega; \quad \partial_n G_h = 0, \quad x \in \partial\Omega, \tag{3.50 a}$$

$$G_h(x;x_0,\lambda^*) \sim -\frac{1}{2\pi}\log|x - x_0| + R_h(x_0;x_0,\lambda^*) + o(1), \quad \text{as} \quad x \to x_0. \tag{3.50 b}$$

In terms of this Green's function, $u^*(x,\nu)$ is given by

$$u^*(x,\nu) = -2\pi\, A\,\nu\, G_h(x;x_0,\lambda^*).$$

By using (3.50 b), we expand u^* as $x \to x_0$ to obtain

$$u^*(x,\nu) \sim A\,\nu\, \log|x - x_0| - 2\pi\, A\,\nu\, R_h(x_0;x_0,\lambda^*), \quad \text{as} \quad x \to x_0. \tag{3.51}$$

The matching condition is that the expressions in (3.49) and (3.51) agree. The $\log|x - x_0|$ terms agree automatically, and from the remaining terms, we obtain a transcendental equation for $\lambda^*(\nu)$ given by

$$R_h(x_0;x_0,\lambda^*) = -\frac{1}{2\pi\nu}. \tag{3.52}$$

To obtain the asymptotic behavior for λ_0, we need the solution λ^* of (3.52) that tends to zero as $\nu \to 0$.

Equation (3.52) can, in general, only be solved numerically as a function of ν. Below, we only determine an expression for λ^* that is correct to terms of order $\mathcal{O}(\nu^2)$. To obtain this expression, we expand the Helmholtz Green's function, $G_h(x;x_0,\lambda^*)$, in terms of $\lambda^* \ll 1$, as

$$G(x;x_0,\lambda^*) = \frac{1}{\lambda^*}G_0(x;x_0) + G_1(x;x_0) + \lambda^* G_2(x;x_0) + \cdots. \tag{3.53}$$

Substituting (3.53) into (3.50), we get a series of problems for the $G_j(x;x_0)$, $j=0,1,2,\ldots$. At order $\mathcal{O}(1/\lambda^*)$, G_0 satisfies $\Delta G_0 = 0$ in Ω and $\partial_n G_0 = 0$ on $\partial\Omega$, from which we obtain that G_0 is a constant. The higher-order corrections G_j for $j \geq 1$ are readily found to satisfy

$$\Delta G_j = \begin{cases} -\delta(x-x_0) - G_0, & j=1, \\ -G_{j-1}, & j>1, \end{cases} \qquad x \in \Omega\,; \quad \partial_n G_j = 0, \quad x \in \partial\Omega\,, \quad j \geq 1\,; \quad \int_\Omega G_j\, dx = 0, \quad j \geq 1\,. \tag{3.54}$$

Applying the Divergence Theorem, we obtain that $G_0 = -1/|\Omega|$, where $|\Omega|$ is the area of Ω. The function $G_1(x;x_0)$ (which we shall henceforth call G_N) is the Neumann Green's function, with regular part $R_N(x_0;x_0)$ defined by

$$\Delta G_N = \frac{1}{|\Omega|} - \delta(x-x_0)\,, \quad x \in \Omega\,, \tag{3.55 a}$$

$$\partial_n G_N = 0\,, \quad x \in \partial\Omega\,, \tag{3.55 b}$$

$$\int_\Omega G_N\, dx = 0\,. \tag{3.55 c}$$

We notice that $G_N(x;x_0)$ exists since $\int_\Omega \left(\frac{1}{|\Omega|} - \delta(x-x_j) \right) dx = 0$, and is unique due to the constraint $\int_\Omega G_N(x;x_0)\, dx = 0$. In addition, we can decompose $G_N(x;x_j)$ as

$$G_N(x;x_0) = -\frac{1}{2\pi} \log|x-x_0| + R_N(x;x_0)\,, \tag{3.55 d}$$

where $R_N(x;x_0)$ is the regular (smooth) part of the Neumann Green's function.

From (3.53) and (3.55), we write the two-term expansion for G when $\lambda^* \ll 1$ as

$$G_h(x;x_0,\lambda^*) = -\frac{1}{|\Omega|\lambda^*} + G_N(x;x_0) + \mathcal{O}(\lambda^*)\,. \tag{3.56}$$

A similar two-term expansion for the regular part R_h of the Helmholtz Green's function in terms of the regular part of the Neumann Green's function is

$$R_h(x_0;x_0,\lambda^*) = -\frac{1}{|\Omega|\lambda^*} + R_N(x_0;x_0) + \mathcal{O}(\lambda^*)\,. \tag{3.57}$$

Substituting this expression into (3.52), we get the following two-term asymptotic result:

Principal Result 3.2:(One Hole) *For $\varepsilon \to 0$, the first eigenvalue λ_0 of (3.41) has the two-term asymptotic behavior*

$$\lambda_0(\varepsilon) = \frac{2\pi\nu}{|\Omega|\,(1 + 2\pi\nu R_N(x_0;x_0))} + \mathcal{O}(\nu^3) = \frac{2\pi\nu}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|} R_N(x_0;x_0) + \mathcal{O}(\nu^3)\,. \tag{3.58}$$

Here $\nu = -1/\log(\varepsilon d)$, and d is the logarithmic capacitance determined from the inner problem (3.45). An infinite-order logarithmic expansion for λ_0 is given by $\lambda_0 \sim \lambda^*$, where λ^* is the first positive root of (3.52).

Next, we extend the asymptotic framework to the case of K holes. Much of the analysis above remains the same, except that now the single hole x_0 is replaced by x_i, for $i = 1, \ldots, K$. The hybrid formulation for K holes is

$$\Delta u^* + \lambda^* u^* = 0\,, \quad x \in \Omega\backslash\{x_1, \ldots, x_K\}\,; \quad \int_\Omega (u^*)^2\, dx = 1\,; \quad \partial_n u^* = 0\,, \quad x \in \partial\Omega\,, \tag{3.59 a}$$

$$u^* \sim A_i\, \nu_i\, \log|x-x_i| + A_i\,, \quad \text{as} \quad x \to x_i\,, \quad i = 1, \ldots, K\,. \tag{3.59 b}$$

Here, $\nu_i = -1/\log(\varepsilon d_i)$, where d_i is the logarithmic capacitance of the i^{th} hole. In this formulation, we have the K unknowns, A_i, for $i = 1, \ldots, K$, and one normalization condition for u^*. The normalization condition effectively sets one relation between the A_i, for $i = 1, \ldots, K$.

We write u^* in terms of the Helmholtz Green's function defined in (3.50), and then take the limit $x \to x_i$ to get

$$u^* = -2\pi \sum_{j=1}^{K} A_j \nu_j G_h(x; x_j, \lambda^*) \sim A_i \nu_i \left(\log|x - x_i| - 2\pi\nu_i R_h(x_i; x_i, \lambda^*)\right) - 2\pi \sum_{\substack{j=1 \\ j\neq i}}^{K} A_j \nu_j G_h(x_i; x_j, \lambda^*)\,. \tag{3.60}$$

The matching condition is that the expressions in (3.59 b) and (3.60) agree. The logarithmic terms agree, and from the remaining terms, we obtain a $K \times K$ homogeneous linear system to solve for the A_i

$$A_i \left(1 + 2\pi\nu_i R_h(x_i; x_i, \lambda^*)\right) + 2\pi \sum_{\substack{j=1 \\ j\neq i}}^{K} A_j \nu_j G_h(x_i; x_j, \lambda^*) = 0\,, \quad i = 1, \ldots, K\,. \tag{3.61}$$

A solution to (3.61) exists only when the following determinant vanishes:

$$\begin{vmatrix} (1 + 2\pi\nu_1 R_{h11}(\lambda^*)) & 2\pi\nu_2 G_{h12}(\lambda^*) & \cdots & 2\pi\nu_K G_{h1K}(\lambda^*) \\ 2\pi\nu_1 G_{h21}(\lambda^*) & (1 + 2\pi\nu_2 R_{h22}(\lambda^*)) & & \vdots \\ \vdots & & \ddots & \\ 2\pi\nu_1 G_{hK1}(\lambda^*) & \cdots & 2\pi\nu_{K-1} G_{hKK-1}(\lambda^*) & (1 + 2\pi\nu_K R_{hKK}(\lambda^*)) \end{vmatrix} = 0\,. \tag{3.62}$$

Here we have defined $R_{hii}(\lambda^*) = R_h(x_i; x_i, \lambda^*)$, $G_{hij}(\lambda^*) = G_h(x_i; x_j, \lambda^*)$, for $i \neq j$, and $\nu_i = -1/\log(\varepsilon d_i)$ for $i = 1, \ldots, K$. We need the solution $\lambda^*(\nu_1, \ldots, \nu_K)$ of (3.62) that tends to zero as $\nu_i \to 0$ for $i = 1, \ldots, K$. Equation (3.62) provides an expression for $\lambda^*(\nu_1, \ldots, \nu_K)$ that sums all the logarithmic terms in the asymptotic expansion of $\lambda_0(\varepsilon)$.

As with the case for one hole in the domain, we can derive an asymptotic formula for λ^* that has an error of $\mathcal{O}(\nu^3)$. This formula is again determined in terms of the Neumann Green's function G_N and its regular part R_N, defined in (3.55). By using (3.56) and (3.57) in (3.62), we obtain a homogeneous linear system for the A_i

$$A_i \left[1 + 2\pi\nu_i R_N(x_j; x_j) - \frac{2\pi\nu_i}{|\Omega|\lambda^*}\right] + 2\pi \sum_{\substack{j=1 \\ j\neq i}}^{K} A_j \nu_j \left[-\frac{1}{|\Omega|\lambda^*} + G_N(x_j; x_i)\right] = 0\,, \quad i = 1, \ldots, K\,. \tag{3.63}$$

It is convenient to write (3.63) in matrix form as

$$\mathcal{C}\boldsymbol{a} = \frac{2\pi}{|\Omega|\lambda^*} \mathcal{B}\mathcal{V}\boldsymbol{a}\,; \quad \mathcal{V} \equiv \begin{pmatrix} \nu_1 & 0 & \cdots & 0 \\ 0 & \ddots & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \nu_K \end{pmatrix}, \quad \mathcal{B} \equiv \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & \ddots & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}, \quad \boldsymbol{a} \equiv \begin{pmatrix} A_1 \\ \vdots \\ A_K \end{pmatrix}. \tag{3.64 a}$$

In (3.64 a), the matrix $\mathcal{C}$ is defined in terms of the Neumann Green's function matrix $\mathcal{G}_N$ by

$$\mathcal{C} = I + 2\pi\mathcal{G}_N\mathcal{V}\,, \tag{3.64 b}$$

where

$$\mathcal{G}_N \equiv \begin{pmatrix} R_N(x_1; x_1) & G_N(x_1; x_2) & \cdots & \cdots & G_N(x_1; x_K) \\ G_N(x_2; x_1) & R_N(x_2; x_2) & G_N(x_2; x_3) & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \cdots & \cdots & G_N(x_{K-1}; x_{K-2}) & R_N(x_{K-1}; x_{K-2}) & G_N(x_{K-1}; x_K) \\ G_N(x_K; x_1) & \cdots & \cdots & G_N(x_K; x_{K-1}) & R_N(x_K; x_K) \end{pmatrix}. \tag{3.64 c}$$

Let $\nu_m = \max_{j=1,\ldots,K} \nu_j$. Then, for ν_m sufficiently small, we can invert $\mathcal{C}$, to obtain that λ^* is an eigenvalue of the matrix eigenvalue problem

$$\mathcal{A}\boldsymbol{a} = \lambda^* \boldsymbol{a}\,, \qquad \mathcal{A} = \frac{2\pi}{|\Omega|}\mathcal{C}^{-1}\mathcal{B}\mathcal{V}\,. \tag{3.65}$$

By using this representation of λ^* we obtain the following result:

Principal Result 3.3:(**K Holes**) *For $\varepsilon \to 0$, the first eigenvalue λ_0 of (3.41) has the explicit two-term asymptotic behavior*

$$\lambda_0(\varepsilon) \sim \lambda^*\,, \qquad \lambda^* = \frac{2\pi}{|\Omega|}\left(\sum_{j=1}^{K}\nu_j - 2\pi\sum_{j=1}^{K}\sum_{i=1}^{K}\nu_j\nu_i\left(\mathcal{G}\right)_{Nij}\right) + \mathcal{O}(\nu_m^3)\,. \tag{3.66}$$

Here $\left(\mathcal{G}\right)_{Nij}$ are the entries of the Neumann Green's function matrix $\mathcal{G}_N$ defined in (3.64 c).

Proof: We first notice that the matrix $\mathcal{B}\mathcal{V}$ has rank one, since $\mathcal{V}$ is diagonal and $\mathcal{B} = \boldsymbol{e}_0\boldsymbol{e}_0^t$, where $\boldsymbol{e}_0^t = (1, 1, \ldots, 1)$. This implies that $\mathcal{A}$ has rank one, and so λ^* is the unique nonzero eigenvalue of $\mathcal{A}$. Hence, $\lambda^* = \text{Trace}\mathcal{A}$. By using the structure of $\mathcal{A}$ in (3.65), we readily calculate that

$$\lambda^* = \frac{2\pi}{|\Omega|}\sum_{j=1}^{K}\nu_j\left(\sum_{i=1}^{K}c_{ij}\right)\,, \qquad c_{ij} \equiv \left(\mathcal{C}^{-1}\right)_{ij}\,. \tag{3.67}$$

Finally, we use the asymptotic inverse $\mathcal{C}^{-1} \sim I - 2\pi\mathcal{G}_N\mathcal{V} + \cdots$ for $\nu_m \ll 1$ to calculate c_{ij}. Substituting this result into (3.67) we obtain (3.66). ■

As a Corollary to this result, we obtain the following simplification for the case of K identical holes:

Corollary:(**K Identical Holes**) *Suppose that the K holes are identical, in the sense that εd_j is independent of j. Then, (3.66) can be written as the explicit two-term expansion*

$$\lambda_0(\varepsilon) \sim \lambda^*\,, \qquad \lambda^* = \frac{2\pi K\nu}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|}p(x_1, \ldots, x_K) + \mathcal{O}(\nu^3)\,, \tag{3.68}$$

where $\nu \equiv -1/\log(\varepsilon d)$, and the function $p(x_1, \ldots, x_K)$ is defined by

$$p(x_1, \ldots, x_K) = \sum_{j=1}^{K}\sum_{i=1}^{K}\left(\mathcal{G}\right)_{Nij} \equiv K\boldsymbol{e}^t\mathcal{G}_N\boldsymbol{e} = \sum_{i=1}^{K}\left(R_N(x_i; x_i) + \sum_{\substack{j=1\\ j\neq i}}^{K}G_N(x_j; x_i)\right)\,. \tag{3.69}$$

Here $\left(\mathcal{G}\right)_{Nij}$ are the entries in the matrix $\mathcal{G}_N$ in (3.64 c), and $\boldsymbol{e}$ is the unit vector $\boldsymbol{e} = K^{-1/2}(1, .., 1)^T$. For K circular holes of radius ε, then $d_j = 1$ for $j = 1, \ldots, K$, and so $\nu = -1/\log\varepsilon$.

When Ω is the unit disk, the optimal spatial configurations of the centers $\{x_1, \ldots, x_K\}$ of K distinct traps of a common radius ε were computed numerically in [**38**] by optimizing the function $p(x_1, \ldots, x_K)$ in (3.69). For the unit disk, the Neumann Green's function $G_N(x; \xi)$ and its regular part $R_N(\xi; \xi)$ are explicitly available, and are given by

$$G(x; x_0) = \frac{1}{2\pi}\left(-\log|x - x_0| - \log\left|x|x_0| - \frac{x_0}{|x_0|}\right| + \frac{1}{2}(|x|^2 + |x_0|^2) - \frac{3}{4}\right)\,, \tag{3.70 a}$$

$$R(x_0; x_0) = \frac{1}{2\pi}\left(-\log\left|x_0|x_0| - \frac{x_0}{|x_0|}\right| + |x_0|^2 - \frac{3}{4}\right)\,. \tag{3.70 b}$$

By using this Green's function, it is readily shown that the problem of minimizing the function $p(x_1, \ldots, x_K)$ is equivalent to the discrete variational problem of minimizing the function $\mathcal{F}(x_1, \ldots, x_K)$ defined by

$$\mathcal{F}(x_1, \ldots, x_K) = -\sum_{j=1}^{K} \sum_{\substack{k=1 \\ k \neq j}}^{K} \log |x_j - x_k| - \sum_{j=1}^{K} \sum_{k=1}^{K} \log |1 - x_j \bar{x}_k| + K \sum_{j=1}^{K} |x_j|^2 \,, \quad |x_j| < 1 \,, \tag{3.71}$$

for $x_j \neq x_k$ when $j \neq k$, and where $\bar{x}_k$ denotes the complex conjugate of x_k.

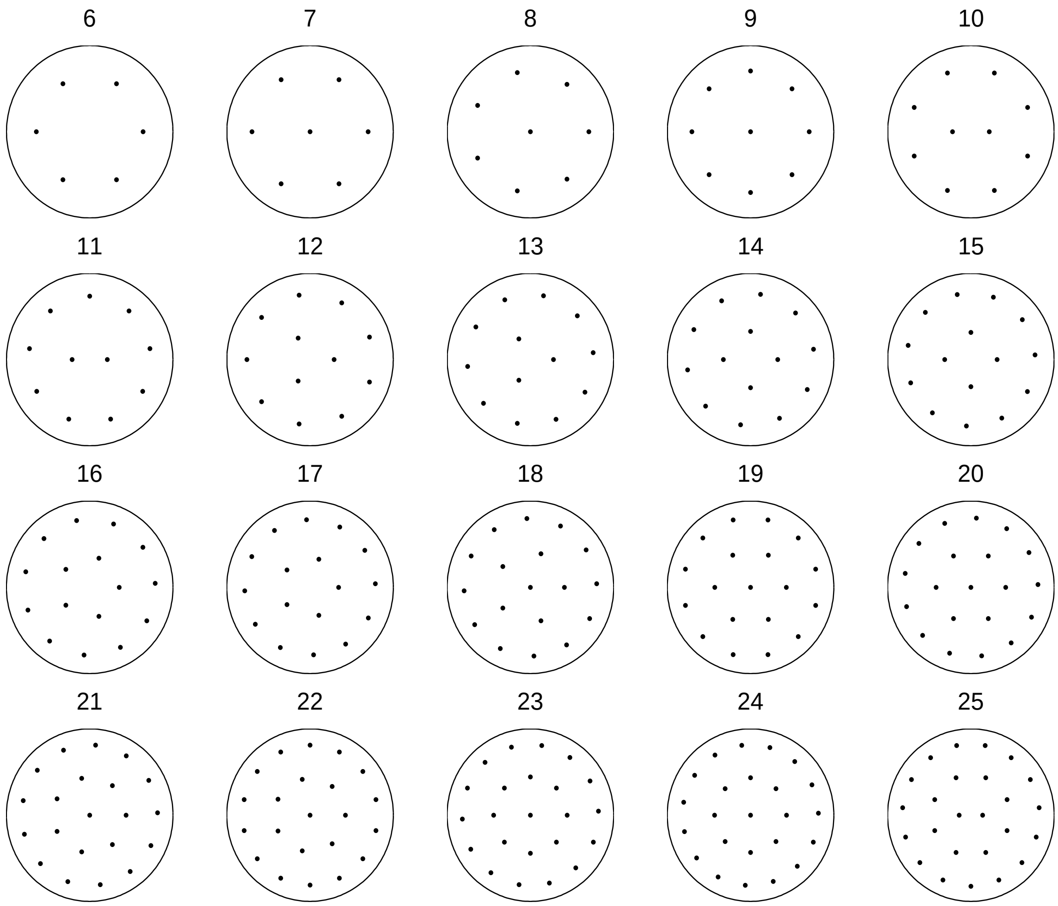


FIGURE 4. Optimum configuration of $6 \leq K \leq 25$ traps inside the unit disk that minimizes the principal eigenvalue of (3.41).

For K small, optimal patterns consist of ring arrangements of traps, which can be analyzed explicitly as in [**38**]. The optimal patterns of holes for $6 \leq K \leq 25$ are shown in Fig. 4. An interesting open problem is to determine the optimal arrangement of $K \gg 1$ traps in the dilute fraction limit $K\pi\varepsilon^2 \ll 1$, and to determine a scaling law valid for $N \gg 1$ for the optimal energy $\mathcal{F}$. In particular, does the optimal arrangement approach a hexagonal lattice structure with a boundary layer near the rim of the unit disk? Can the limiting result for the eigenvalue asymptotics be predicted from the dilute fraction limit of homogenization theory?

As this stage the reader should attempt the following two problems (the solutions are given in Appendix B):

Problem 3.3: *Consider the principal eigenvalue of (3.41) in the unit disk, with the Dirichlet condition $u = 0$ posed on $\partial\Omega$ instead of $\partial_n u = 0$ on $\partial\Omega$. Assume that there is one arbitrarily-shaped hole centered at the origin of the unit disk. Derive an explicit transcendental equation for the infinite-order logarithmic series approximation to the* *principal eigenvalue, and apply your result to the special case of the unit disk that contains a hole of arbitrary shape centered at the origin.*

Problem 3.4: *Consider (3.41) for the case of K holes that have a common logarithmic capacitance $d = d_1 = \ldots, d_K$. By introducing two-term expansions directly in (3.41) for the eigenvalue and for the outer and inner approximations to the eigenfunction, re-derive the two-term approximation given in (3.68) of the Corollary.*

3.4 The Fundamental Eigenvalue on the Surface of a Sphere with Localized Traps

A related spectral problem concerns the determination of the mean first passage time (MFPT) for Brownian motion on the surface of the unit sphere S in the presence of a collection of perfectly absorbing traps of asymptotically small radii. This problem, with clear biophysical applications, was studied in [**19**]. In this context, the average MFPT is asymptotically proportional to the inverse of the principal eigenvalue $\sigma^\star(\varepsilon)$ of the Laplace-Beltrami operator for the sphere. The eigenvalue problem is formulated as

$$\triangle_s \psi + \sigma \psi = 0 \,, \quad x \in S_\varepsilon \equiv S \backslash \cup_{j=1}^{K} \Omega_{\varepsilon_j} \,; \quad \psi = 0 \,, \quad x \in \partial \Omega_{\varepsilon_j} \,, \quad j = 1, \ldots, N \,. \tag{3.72}$$

Each trap is assumed to be centered at some $x_j \in S$ with $|x_j| = 1$ and has radius $\mathcal{O}(\varepsilon)$, with $\varepsilon \ll 1$. The traps are assumed to be well-separated in the sense that $|x_i - x_j| = \mathcal{O}(1)$ for $i \neq j$ and $i, j = 1, \ldots, K$. In (3.72), Δ_s is the Laplace-Beltrami operator for the sphere.

We consider the special case of K locally circular traps of a common radius ε. Then, the principal eigenvalue $\sigma^\star(\varepsilon)$ has an infinite logarithmic expansion of the form $\sigma(\varepsilon)$ as

$$\sigma^\star(\varepsilon) = \mu \sigma_0 + \mu^2 \sigma_1 + \mu^3 \sigma_2 + \cdots \,, \qquad \mu \equiv -\frac{1}{\log \varepsilon} \,. \tag{3.73}$$

The logarithmic nature of the expansion is similar to other problems in two space dimensions with localized perturbations (cf. [**6**], [**38**], [**70**], and [**77**]). One can readily derive a two-term expansion for this principal eigenvalue as in [**19**] by deriving simple formulae for the coefficients σ_0 and σ_1. Since the curvature of the sphere provides only an $\mathcal{O}(\varepsilon)$ correction to the solution in the inner region near each trap, this contribution is asymptotically insignificant in comparison with the logarithmic gauge $-1/\log \varepsilon$. Consequently, the curvature of the sphere can be neglected in each inner region. The two-term result from [**19**] is summarized as follows:

Principal Result 3.4: *Consider (3.72) for K circular traps of a common radius ε centered at x_j, for $j = 1, \ldots, N$, on the unit sphere. Then, the principal eigenvalue $\sigma^\star(\varepsilon)$ of (3.72) has the two-term asymptotic expansion*

$$\sigma(\varepsilon) \sim \frac{\mu K}{2} + \mu^2 \left[-\frac{K^2}{4} \left(2 \log 2 - 1 \right) + p(x_1, \ldots, x_K) \right] \,, \qquad \mu \equiv -\frac{1}{\log \varepsilon} \,, \tag{3.74}$$

where $p(x_1, \ldots, x_K)$ is the discrete energy defined by

$$p(x_1, \ldots, x_K) \equiv \sum_{i=1}^{K} \sum_{j>i}^{K} \log |x_i - x_j| \,. \tag{3.75}$$

This result shows that the optimal configuration $\{x_1, \ldots, x_K\}$ of the centers of the traps that maximize the fundamental eigenvalue, thereby minimizing the lifetime of the wandering Brownian particle, is at the so-called elliptic Fekete points that minimize the discrete logarithmic energy $-\sum_{i=1}^{K}\sum_{j>i}^{K}\log|x_i - x_j|$ on the unit sphere. This famous discrete variational problem has a long history in approximation theory (see [**5**], [**27**], [**55**]).

The derivation of the main result (3.74) involves, in a rather central way, the modified Green's function $G_m(x;x_0)$ for the sphere, defined as the unique solution to

$$\triangle_s G_m = \frac{1}{4\pi} - \delta(x-x_0)\,, \quad x \in S\,, \tag{3.76 a}$$

$$G_m \quad \text{is } 2\pi \text{ periodic in } \phi \text{ and smooth at } \theta = 0,\pi\,, \tag{3.76 b}$$

$$\int_S G_m\, ds \equiv \int_0^{2\pi}\int_0^{\pi} G_m \,\sin\theta\, d\theta d\phi = 0\,. \tag{3.76 c}$$

Here x and x_0 are given in terms of spherical coordinates ϕ (longitude) and θ (latitude) by

$$x = (\cos\phi\sin\theta,\, \sin\phi\sin\theta,\, \cos\theta)\ , \qquad x_0 = (\cos\phi_0\sin\theta_0,\, \sin\phi_0\sin\theta_0,\, \cos\theta_0)\ . \tag{3.77}$$

The solution of (3.76) is well-known from various studies of the motion of fluid vortices on the sphere (see [**36**] and the references therein), and is given explicitly for any $x \in S$ by

$$G_m(x;x_0) = -\frac{1}{2\pi}\log|x-x_0| + R_m\,, \qquad R_m \equiv \frac{1}{4\pi}\left[2\log 2 - 1\right]\,, \tag{3.78}$$

where R_m is the (constant) regular part of G_m.

To formulate a problem that has the effect of summing all of the logarithmic terms in the asymptotic expansion of (3.72), we do not expand ψ or $\sigma^\star(\varepsilon)$ in an infinite logarithmic series. Instead, we take the outer solution for ψ to satisfy (3.72) in the punctured domain $S\backslash\{x_1,\ldots,x_K\}$, with an appropriate singularity behavior at each x_j that asymptotically matches with the inner solution to Laplace's equation. In this way, the hybrid asymptotic-numerical formulation for the outer solution for ψ and the eigenvalue σ is to solve

$$\triangle_s\psi + \sigma\psi = 0\,, \quad x \in S\backslash\{x_1,\ldots,x_K\}\,, \tag{3.79 a}$$

$$\psi \sim A_j + \mu_j A_j \log|x-x_j|\,, \quad \text{as} \quad x \to x_j\,, \quad j = 1,\ldots,K\,. \tag{3.79 b}$$

with $\int_S \psi^2\, ds = 1$, where ψ is singularity-free at the poles $\theta = 0,\pi$ and is 2π periodic in ϕ.

To represent the solution to (3.79), we first must introduce the Helmholtz Green's function $G_H(x;x_0,\nu)$ for the Laplace-Beltrami operator, defined as the solution to

$$\triangle_s G_H + \nu(\nu+1)G_H = -\delta(x-x_0)\,, \quad x \in S\,, \tag{3.80 a}$$

$$G_H \quad \text{is } 2\pi \text{ periodic in } \phi \text{ and smooth at } \theta = 0,\pi\,. \tag{3.80 b}$$

This Green's function, which arises in the study of high frequency wave scattering (see [**69**] and [**73**]), is given explicitly by

$$G_H(x;x_0,\nu) = -\frac{1}{4\sin(\pi\nu)}P_\nu\left(-x\cdot x_0\right)\,, \tag{3.81}$$

where $P_\nu(z)$ is the Legendre function of the first kind of order ν. As $z \to -1$, it follows from [**23**] that

$$P_\nu(z) \sim \frac{\sin(\pi\nu)}{\pi}\left[\log\left(\frac{1+z}{2}\right) + 2\gamma_e + 2\psi(\nu+1) + \pi\cot(\pi\nu)\right]\,, \tag{3.82}$$

where $\psi(z)$ is the psi or digamma function, which is defined in terms of the Gamma function $\Gamma(z)$ by (cf. [**23**])

$$\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} = \log z + \int_0^\infty e^{-zt}\left(\frac{1}{t} - \frac{1}{1-e^{-t}}\right) dt\,. \tag{3.83}$$

Here γ_e is Euler's constant. Upon substituting (3.82) into (3.81), and recalling that $1 - x\cdot x_0 = |x-x_0|^2/2$, we readily obtain that as $x \to x_0$ the Helmholtz Green's function has the local behavior

$$G_H(x;x_0,\nu) = -\frac{1}{2\pi}\log|x-x_0| + R_h(\nu) + o(1)\,, \quad \text{as } \; x \to x_0\,,$$
$$R_H(\nu) \equiv -\frac{1}{4\pi}\left[-2\log 2 + 2\gamma_e + 2\psi(\nu+1) + \pi\cot(\pi\nu)\right]\,. \tag{3.84 a}$$

This local expansion identifies the constant regular part $R_H(\nu)$ of this Green's function.

The solution to (3.79) is then written as

$$\psi = -2\pi\mu\sum_{i=1}^{K} A_i G_H(x;x_i,\nu)\,. \tag{3.85}$$

Then, by using (3.84 a), we can expand ψ as $x \to x_j$ for each $j = 1,\ldots,K$ to obtain

$$\psi \sim \mu A_j \log|x-x_j| - 2\pi\mu A_j R_H - 2\pi\mu \sum_{\substack{i=1\\ i\neq j}}^{K} A_i G_{Hji}\,, \quad \text{as} \quad x \to x_j\,. \tag{3.86}$$

By comparing (3.86) with the required singular behavior (3.79 b), we conclude that A_j must satisfy the following homogeneous linear system:

$$A_j + 2\pi\mu A_j R_H + 2\pi\mu\sum_{\substack{i=1\\ i\neq j}}^{K} A_i G_{Hji} = 0\,, \qquad j = 1,\ldots,K\,. \tag{3.87}$$

Here $G_{Hji} = G_H(x_j;x_i,\nu)$ is given in terms of $\sigma = \nu(\nu+1)$ by (3.81). We seek the smallest value of $\sigma(\varepsilon)$ for which (3.87) has a nontrivial solution. This smallest value, denoted by $\sigma^*(\varepsilon)$ is the infinite-order logarithmic approximation to the fundamental eigenvalue. The corresponding eigenvector $A_1,\ldots,A_K$ is determined up to a scalar multiple. This scalar multiple can then be found by substituting (3.85) into the normalization condition $\int_S \psi^2\, ds = 1$. This leads to the following result:

Principal Result 3.5: *Consider (3.72) for K locally circular traps of common radius ε, and define $\mu \equiv -1/\log\varepsilon$. Then, with an error of order $\mathcal{O}(\varepsilon\mu)$, the principal eigenvalue $\sigma(\varepsilon)$ of (3.72) is the smallest root of the transcendental equation*

$$\mathrm{Det}\left(I + 2\pi\mu\left(R_h I + \mathcal{G}_H\right)\right) = 0\,. \tag{3.88 a}$$

Here I is the $K\times K$ identity matrix, while $\mathcal{G}_H$ is the Helmholtz Green's function matrix with matrix entries

$$\mathcal{G}_{Hjj} = 0\,, \quad j = 1,\ldots,K\,; \qquad \mathcal{G}_{Hij} = -\frac{1}{4\sin(\pi\nu)} P_\nu\left(\frac{|x_j-x_i|^2}{2} - 1\right)\,, \quad i \neq j\,, \tag{3.88 b}$$

where $P_\nu(z)$ is the Legendre function of the first kind of order ν.

We remark that both R_H, given in (3.84 a), and $\mathcal{G}_{Hij}$ depend on ν. Therefore, we must solve (3.88) numerically for $\nu = \nu(\varepsilon)$, which determines $\sigma(\varepsilon)$ from the relation $\sigma = \nu(\nu+1)$.

For the special case of one trap $K = 1$, (3.88) reduces to the transcendental equation $2\pi R_H = -1/\mu$, identical in

	$K = 5$ traps			$K = 2$ traps		
ε	σ	σ^*	σ_2	σ	σ^*	σ_2
0.02	0.7918	0.7894	0.7701	0.2458	0.2451	0.2530
0.05	1.1003	1.0991	1.0581	0.3124	0.3121	0.3294
0.1	1.5501	1.5452	1.4641	0.3913	0.3903	0.4268
0.2	2.5380	2.4779	2.3278	0.5177	0.5110	0.6060

Table 4. Smallest eigenvalue of (3.72) for either two or five equally-spaced circular traps of a common radius ε on the surface of the unit sphere. Here, σ is the numerical solution found by COMSOL [**17**], $\sigma^* = \nu(1+\nu)$ corresponds to the root ν of the transcendental equation (3.88 *a*), and σ_2 is calculated from the two-term expansion (3.74).

form to that in (3.52) for the planar domain. By using (3.84 *a*) for R_H, we obtain that that the approximation to $\sigma(\varepsilon)$ that accounts for all the logarithmic terms in the expansion is the smallest root of

$$-\log 2 + \gamma_e + \psi(\nu+1) + \frac{\pi}{2}\cot(\pi\nu) = \frac{1}{\mu}\,, \qquad \sigma = \nu + \nu^2\,, \tag{3.89}$$

where γ_e is Euler's constant, and $\psi(z)$ is the digamma function defined in (3.83). We can readily recover the two-term expansion (3.74) for $N = 1$ by substituting $\psi(\nu+1) \sim -\gamma_e$ and $\pi\cot\pi\nu \sim 1/\nu$ for $\nu \ll 1$ into (3.89) and then solving for σ.

To validate the asymptotic result in (3.88), we used the eigenvalue solver of the COMSOL software package [**17**] to compute the smallest eigenvalue, together with the corresponding eigenmode, of (3.72) for both a 2- and a 5-trap configuration with equally spaced traps on the unit sphere. The two-term results, the infinite-logarithmic expansion results, and the full numerical results, are shown in Table 4. From this table, we observe that for $\varepsilon = 0.2$ and $K = 5$ traps, for which the trap surface area fraction is $f = 5\pi\varepsilon^2/(4\pi)\times 100\% = 5\%$, the infinite-order logarithmic expansion still provides a very close approximation to the full numerical result.

3.5 The Narrow Escape Problem in 2-D Domains

The narrow escape problem in a two-dimensional domain is described as the motion of a Brownian particle confined in a bounded domain $\Omega \in R^2$ whose boundary $\partial\Omega = \partial\Omega_r \cup \partial\Omega_a$ is almost entirely reflecting ($\partial\Omega_r$), except for small absorbing windows, labeled collectively by $\partial\Omega_a$, through which the particle can escape (see Fig. 5). Denoting the trajectory of the Brownian particle by $X(t)$, the mean first passage time (MFPT) $v(x)$ is defined as the expectation value of the time τ taken for the Brownian particle to become absorbed somewhere in $\partial\Omega_a$ starting initially from $X(0) = x \in \Omega$, so that $v(x) = E[\tau \,|\, X(0) = x]$. The calculation of $v(x)$ becomes a narrow escape problem in the limit when the measure of the absorbing set $|\partial\Omega_a| = \mathcal{O}(\varepsilon)$ is asymptotically small, where $0 < \varepsilon \ll 1$ measures the dimensionless radius of an absorbing window.

Narrow escape problems have many biophysical applications (cf. [**62**], [**66**]). In this context, the Brownian particles could be diffusing ions, globular proteins or cell-surface receptors. It is then of interest to determine, for example, the mean time that an ion requires to find an open ion channel located in the cell membrane or the mean time of a receptor to hit a certain target binding site (cf. [**62**]).

It is well-known (cf. [**62**], [**66**]) that the MFPT $v(x)$ satisfies a Poisson equation with mixed Dirichlet-Neumann boundary conditions, formulated as

$$\triangle v = -\frac{1}{D}\,, \quad x \in \Omega\,, \tag{3.90 a}$$

$$v = 0\,, \quad x \in \partial\Omega_a = \cup_{j=1}^{N} \partial\Omega_{\varepsilon_j}\,, \quad j = 1, \ldots, N\,; \quad \partial_n v = 0\,, \quad x \in \partial\Omega_r\,, \tag{3.90 b}$$

where D is the diffusion coefficient associated with the underlying Brownian motion. In (3.90), the absorbing set consists of N small disjoint absorbing windows $\partial\Omega_{\varepsilon_j}$ centered at $x_j \in \partial\Omega$ (see Fig. 5). In our two-dimensional setting, we assume that the length of each absorbing arc is $|\partial\Omega| = \varepsilon l_j$, where $l_j = \mathcal{O}(1)$ for $j = 1, \ldots, N$. It is further assumed that the windows are well-separated in the sense that $|x_i - x_j| = \mathcal{O}(1)$ for all $i \neq j$. With respect to a uniform distribution of initial points $x \in \Omega$, the average MFPT, denoted by $\bar{v}$, is defined by

$$\bar{v} = \chi \equiv \frac{1}{|\Omega|} \int_\Omega v(x)\, dx\,, \tag{3.91}$$

where $|\Omega|$ denotes the area of Ω.

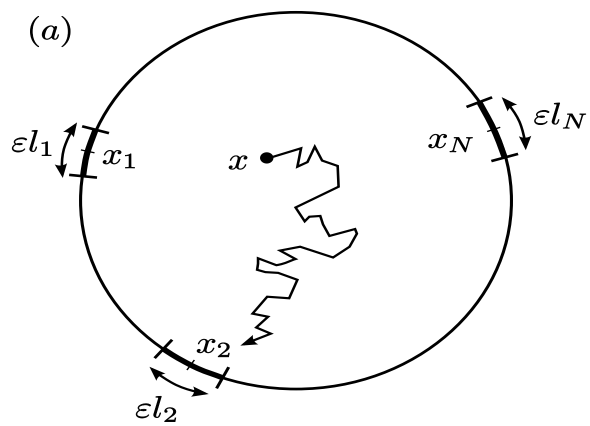


FIGURE 5. Sketch of a Brownian trajectory in the two-dimensional unit disk with absorbing windows on the boundary

Since the MFPT diverges as $\varepsilon \to 0$, the calculation of the MFPT $v(x)$, and that of the average MFPT $\bar{v}$, constitutes a singular perturbation problem. The asymptotic solution to this problem as constructed in [**53**], and summarized below, involves an infinite logarithmic expansion.

To construct the inner solution near the j^{th} absorbing arc, we write (3.90) in terms of a local orthogonal coordinate system where η denotes the distance from $\partial\Omega$ to $x \in \Omega$, and s denotes arclength on $\partial\Omega$. In terms of these coordinates, the problem (3.90 a) for $v(x)$ transforms to the following problem for $w(\eta, s)$:

$$\partial_{\eta\eta} w - \frac{\kappa}{1-\kappa\eta}\partial_\eta w + \frac{1}{1-\kappa\eta}\partial_s\left(\frac{1}{1-\kappa\eta}\partial_s w\right) = -\frac{1}{D}\,. \tag{3.92}$$

Here κ is the curvature of $\partial\Omega$ and the center $x_j \in \partial\Omega$ of the j^{th} absorbing arc transforms to $s = s_j$ and $\eta = 0$.

Next, we introduce the local variables $\hat{\eta} = \eta/\varepsilon$ and $\hat{s} = (s - s_j)/\varepsilon$ near the j^{th} absorbing arc. Then, from (3.92) and (3.90 b), we neglect $\mathcal{O}(\varepsilon)$ terms to obtain the inner problem

$$w_{0\hat{\eta}\hat{\eta}} + w_{0\hat{s}\hat{s}} = 0\,, \quad 0 < \hat{\eta} < \infty\,, \quad -\infty < \hat{s} < \infty\,, \tag{3.93 a}$$

$$\partial_{\hat{\eta}} w_0 = 0\,, \quad \text{on } |\hat{s}| > l_j/2\,, \quad \hat{\eta} = 0\,; \quad w_0 = 0\,, \quad \text{on } |\hat{s}| < l_j/2\,, \quad \hat{\eta} = 0\,. \tag{3.93 b}$$

We specify that w_0 has logarithmic growth at infinity, i.e. $w_0 \sim A_j \log|y|$ as $|y| \to \infty$, where A_j is a constant to be determined, and $|y| \equiv \varepsilon^{-1}|x - x_j| = \left(\hat{\eta}^2 + \hat{s}^2\right)^{1/2}$. The solution w_0, unique up to the constant A_j, is readily calculated by introducing elliptic cylinder coordinates in (3.93). It has the far-field behavior

$$w_0 \sim A_j \left[\log|y| - \log d_j + o(1)\right]\,, \quad \text{as} \quad |y| \to \infty\,, \qquad d_j = l_j/4\,. \tag{3.94}$$

In the outer region, the j^{th} absorbing arc shrinks to the point $x_j \in \partial\Omega$ as $\varepsilon \to 0$. With regards to the outer solution, the influence of each absorbing arc is, in effect, determined by a certain singularity behavior at each x_j that results from the asymptotic matching of the outer solution to the far-field behavior (3.94) of the inner solution. In this way, we obtain that the outer solution for v satisfies

$$\triangle v = -\frac{1}{D}\,, \quad x \in \Omega\,; \quad \partial_n v = 0\,, \qquad x \in \partial\Omega \backslash \{x_1, \ldots, x_N\}\,, \tag{3.95 a}$$

$$v \sim \frac{A_j}{\mu_j} + A_j \log|x - x_j|\,, \quad \text{as} \quad x \to x_j\,, \quad j = 1, \ldots, N\,; \qquad \mu_j \equiv -\frac{1}{\log(\varepsilon d_j)}\,, \qquad d_j = \frac{l_j}{4}\,. \tag{3.95 b}$$

Each singularity behavior in (3.95 b) specifies both the regular and singular part of a Coulomb singularity. As such, it provides one constraint for the determination of a linear system for the source strengths A_j for $j = 1, \ldots, N$.

To solve (3.95), we introduce the surface Neumann Green's function $G_s(x;\xi)$ defined as the unique solution of

$$\triangle G_s = \frac{1}{|\Omega|}\,, \qquad x \in \Omega\,; \qquad \partial_n G_s = 0\,, \quad x \in \partial\Omega \backslash \{\xi\}\,, \tag{3.96 a}$$

$$G_s(x;\xi) \sim -\frac{1}{\pi}\log|x - \xi| + R_s(\xi;\xi)\,, \quad \text{as } x \to \xi \in \partial\Omega\,, \tag{3.96 b}$$

$$\int_\Omega G_s(x;\xi)\, dx = 0\,. \tag{3.96 c}$$

Then, the solution to (3.95) is written in terms of $G_s(x;x_j)$ and an unknown constant χ, denoting the spatial average of v, by

$$v = -\pi \sum_{i=1}^{N} A_i G_s(x;x_i) + \chi\,, \qquad \chi = \bar{v} \equiv \frac{1}{|\Omega|}\int_\Omega v\, dx\,. \tag{3.97}$$

To determine a linear algebraic system for A_j, for $j = 1, \ldots, N$, and for χ, we expand (3.97) as $x \to x_j$ and compare it with the required singularity behavior (3.95 b). This yields that

$$A_j \log|x - x_j| - \pi A_j R_{sjj} - \pi \sum_{\substack{i=1 \\ i \neq j}}^{N} A_i G_{sji} + \chi = A_j \log|x - x_j| + \frac{A_j}{\mu_j}\,, \qquad j = 1, \ldots, N\,. \tag{3.98}$$

Here $G_{sji} \equiv G_s(x_j;x_i)$, while $R_{sjj} \equiv R_s(x_j;x_j)$ is the regular part of G_s given in (3.96 b) at $x = x_j$. Equation (3.98) yields N linear equations for χ and A_j, for $j = 1, \ldots, N$. The remaining equation is obtained by noting that

$\triangle v = -\pi \sum_{i=1}^N A_i \triangle G = -\pi |\Omega|^{-1} \sum_{i=1}^N A_i = -D^{-1}$. Thus, the $N+1$ constants χ and A_j, for $j = 1, \ldots, N$, satisfy

$$\frac{A_j}{\mu_j} + \pi A_j R_{sjj} + \pi \sum_{\substack{i=1 \\ i \neq j}}^N A_i G_{sji} = \chi \,, \quad j = 1, \ldots, N \,; \qquad \sum_{i=1}^N A_i = \frac{|\Omega|}{D\pi} \,. \tag{3.99}$$

This linear system of $N+1$ equations can be written in matrix form as

$$\left(I + \pi \mathcal{U} \mathcal{G}_s\right) \mathcal{A} = \chi \mathcal{U} \boldsymbol{e} \,, \qquad \boldsymbol{e}^T \mathcal{A} = \frac{|\Omega|}{D\pi} \,. \tag{3.100}$$

Here $\boldsymbol{e}^T \equiv (1, \ldots, 1)$, $\mathcal{A}^T \equiv (A_1, \ldots, A_N)$, I is the $N \times N$ identity matrix, while the diagonal matrix $\mathcal{U}$ and the symmetric surface Neumann Green's function matrix $\mathcal{G}_s$ are defined by

$$\mathcal{U} \equiv \begin{pmatrix} \mu_1 & 0 & \cdots & 0 \\ 0 & \ddots & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mu_N \end{pmatrix} \,, \qquad \mathcal{G}_s \equiv \begin{pmatrix} R_{s11} & G_{s12} & \cdots & G_{s1N} \\ G_{s21} & R_{s22} & \cdots & G_{s2N} \\ \vdots & \vdots & \ddots & \vdots \\ G_{sN1} & \cdots & G_{sNN-1} & R_{sNN} \end{pmatrix} \,. \tag{3.101}$$

We can then decouple $\mathcal{A}$ and χ in (3.100) to obtain the following main result:

Principal Result 3.6: *Consider N well-separated absorbing arcs for (3.90) of length εl_j for $j = 1, \ldots, N$ centered at $x_j \in \partial\Omega$. Then, the asymptotic solution to (3.90) is given in the outer region $|x - x_j| \gg \mathcal{O}(\varepsilon)$ for $j = 1, \ldots, N$ by*

$$v \sim -\pi \sum_{i=1}^N A_i G_s(x; x_i) + \chi \,. \tag{3.102 a}$$

Here G_s is the surface Neumann Green's function satisfying (3.96), and $\mathcal{A}^T = (A_1, \ldots, A_N)$ is the solution of the linear system

$$\left(I + \pi \mathcal{U} \left(I - \frac{1}{\bar{\mu}} E \mathcal{U}\right) \mathcal{G}_s\right) \mathcal{A} = \frac{|\Omega|}{D\pi N \bar{\mu}} \mathcal{U} \boldsymbol{e} \,, \qquad E \equiv \frac{1}{N} \boldsymbol{e}\boldsymbol{e}^T \,. \tag{3.102 b}$$

In addition, the constant χ, representing the spatial average of v, is given in terms of $\mathcal{A}$, and of μ_j of (3.95 b), by

$$\bar{v} \equiv \chi = \frac{|\Omega|}{D\pi N \bar{\mu}} + \frac{\pi}{N\bar{\mu}} \boldsymbol{e}^T \mathcal{U} \mathcal{G}_s \mathcal{A} \,, \qquad \bar{\mu} \equiv \frac{1}{N} \sum_{j=1}^N \mu_j \,. \tag{3.102 c}$$

Our asymptotic solution to (3.90) in this result has in effect summed all of the logarithmic correction terms in the expansion of the solution, leaving an error that is transcendentally small in ε. Secondly, the constant χ in (3.102 *a*), as given in (3.102 *c*), has the immediate interpretation as the MFPT averaged with respect to an initial uniform distribution of starting points in Ω for the random walk.

For $\mu_j \ll 1$ we can solve (3.102 *b*) and (3.102 *c*) asymptotically by calculating the approximate inverse of the matrix multiplying $\mathcal{A}$ in (3.102 *b*). In this way, we obtain the following two-term result:

Principal Result 3.7: *For $\varepsilon \ll 1$, a two-term expansion for the solution of (3.90) is provided by (3.102 a), where A_j and χ are given explicitly by*

$$A_j \sim \frac{|\Omega| \mu_j}{N D\pi \bar{\mu}} \left(1 - \pi \sum_{i=1}^N \mu_i \mathcal{G}_{sij} + \frac{\pi}{N\bar{\mu}} p_w(x_1, \ldots, x_N)\right) + \mathcal{O}(|\mu|^2) \,, \tag{3.103 a}$$

$$\bar{v} \equiv \chi \sim \frac{|\Omega|}{N D\pi \bar{\mu}} + \frac{|\Omega|}{N^2 D \bar{\mu}^2} p_w(x_1, \ldots, x_N) + \mathcal{O}(|\mu|) \,, \tag{3.103 b}$$

where $|\mu| \equiv \max_{j=1,\ldots,N} \mu_j$. *Here* $p_w(x_1,\ldots,x_N)$ *is the following weighted discrete sum defined in terms of the entries* $\mathcal{G}_{sij}$ *of the surface Neumann Green's function matrix of (3.101):*

$$p_w(x_1,\ldots,x_N) \equiv \sum_{i=1}^{N}\sum_{j=1}^{N} \mu_i \mu_j \mathcal{G}_{sij} \,, \qquad \mu_j = -\frac{1}{\log(\varepsilon d_j)} \,, \quad d_j = \frac{l_j}{4} \,. \tag{3.104}$$

Hence, the average MFPT χ *is minimized for an arrangement of arcs that minimize the discrete sum* $p_w(x_1,\ldots,x_N)$.

We now illustrate the theory for the case where Ω is the unit disk, $\Omega \equiv \{x \,||\, |x| \leq 1\}$. When the singular point is on the boundary of the unit disk, i.e. $\xi \in \partial\Omega$, then the surface Neumann Green's function and its regular part are given explicitly by (cf. [**53**])

$$G_s(x;\xi) = -\frac{1}{\pi}\log|x-\xi| + \frac{|x|^2}{4\pi} - \frac{1}{8\pi} \,, \qquad R_s(\xi;\xi) = \frac{1}{8\pi} \,. \tag{3.105}$$

Consider the special case where N absorbing arcs of a common length 2ε are equally spaced on the boundary of the unit disk. Then, we have that $x_j = e^{2\pi i j/N}$ and $|\partial\Omega_{\varepsilon_j}| = 2\varepsilon$, for $j = 1,\ldots,N$. For this special case, the surface Neumann Green's matrix $\mathcal{G}_s$ is a symmetric circulant matrix, and consequently

$$\mathcal{G}_s \boldsymbol{e} = \frac{p}{N}\boldsymbol{e} \,, \qquad p \equiv p(x_1,\ldots,x_N) \equiv \sum_{i=1}^{N}\sum_{j=1}^{N} \mathcal{G}_{sij} \,, \tag{3.106}$$

where $\boldsymbol{e}^T = (1,\ldots,1)$. For this special case, the exact solution to (3.102 c), which accounts for all logarithmic terms, is

$$\chi = \frac{|\Omega|}{ND\pi\mu} + \frac{|\Omega|}{N^2 D} p(x_1,\ldots,x_N) \,, \qquad \mu = \frac{-1}{\log[(\varepsilon l/4)]} \,. \tag{3.107}$$

Next, by using (3.105) for $G_s(x_i;x_j)$ and $R_s(x_j;x_j)$, we then calculate $p(x_1,\ldots,x_N)$ as

$$\begin{aligned} p(x_1,\ldots,x_N) &= \sum_{k=1}^{N}\sum_{j=1}^{N} \mathcal{G}_{skj} = \frac{N^2}{8\pi} - \frac{1}{\pi}\sum_{k=1}^{N}\sum_{j\neq k}^{N} \log|x_j - x_k| \,, \\ &= \frac{N^2}{8\pi} - \frac{1}{\pi}\sum_{k=1}^{N} \log\left[\prod_{\substack{j=1 \\ j\neq k}}^{N} \left(1 - e^{2\pi i(j-k)/N}\right)\right] = \frac{1}{\pi}\left(\frac{N^2}{8} - N\log N\right) \,, \end{aligned} \tag{3.108}$$

where we have used the simple identity $\prod_{\substack{j=1 \\ j\neq k}}^{N} \left(\alpha - \beta e^{2\pi i(j-k)/N}\right) = |\alpha^{N-1}\left(1 + \frac{\beta}{\alpha} + \cdots + \left(\frac{\beta}{\alpha}\right)^{N-1}\right)|$.

Therefore, for the special case $x_j = e^{2\pi i j/N}$ for $j = 1,\ldots,N$ we obtain from (3.108) and (3.107) that

$$\chi \sim \frac{1}{DN}\left[-\log\left(\frac{\varepsilon N}{2}\right) + \frac{N}{8}\right] \,. \tag{3.109}$$

As remarked following (3.107), the error associated with the asymptotic result (3.109) is smaller than any power of μ. Further examples of the theory are considered in [**19**]. In [**19**] a numerical method is formulated and implemented to numerically compute the surface Neumann Green's function and its regular part numerically for arbitrary bounded two-dimensional domains with smooth boundaries.

3.6 A Nonlinear Problem

In this subsection we show how the method for summing infinite logarithmic expansions can be extended to treat nonlinear elliptic second-order problems on bounded domains.

There are essentially two different ways that nonlinearities can arise. For the first subclass of problems, the outer problem away from the perturbing subdomain is nonlinear, whereas in the vicinity of the hole the problem reduces to Laplace's equation. This is the problem that is considered below. For the second subclass, the inner problem is nonlinear whereas the outer problem is linear. This latter subclass is key to the study of spot solutions to reaction-diffusion systems as discussed in §6.

A model problem of the first type in a bounded two-dimensional domain Ω, which contains a small hole Ω_ε, is

$$\triangle w + F(w) = 0\,, \quad x \in \Omega\backslash\Omega_\varepsilon\,, \tag{3.110 a}$$

$$\partial_n w + b(w - w_b) = 0\,, \quad x \in \partial\Omega\,, \tag{3.110 b}$$

$$w = \alpha\,, \quad x \in \partial\Omega_\varepsilon\,. \tag{3.110 c}$$

Here α is constant, ∂_n denotes the outward normal derivative, $b > 0$, and Ω_ε is a small hole of radius $\mathcal{O}(\varepsilon)$ with $\Omega_\varepsilon \to x_0 \in \Omega$ uniformly as $\varepsilon \to 0$. The function $F(w)$ is assumed to be smooth. Nonlinear problems of this type arise in many applications, including steady-state combustion theory where $F(w)$ is an exponential function (cf. [**77**]). The primary difference between the linear problem (3.10) and the unperturbed problem corresponding to (3.110) is that, depending on the precise nature of the nonlinearity $F(w)$, the unperturbed problem may have no solution, a unique solution, or multiple solutions. We shall assume that the unperturbed problem has at least one solution, and we will focus on determining how a specific solution to this problem is perturbed by the presence of the subdomain Ω_ε.

In the outer region we expand w as in (3.11). The leading-order term $W_0(x;\nu)$ in this expansion satisfies

$$\triangle W_0 + F(W_0) = 0\,, \quad x \in \Omega\backslash\{x_0\}\,, \tag{3.111 a}$$

$$\partial_n W_0 + b(W_0 - w_b) = 0\,, \quad x \in \partial\Omega\,, \tag{3.111 b}$$

$$W_0 \quad \text{is singular as} \;\; x \to x_0\,. \tag{3.111 c}$$

The analysis of the solution in the inner region is the same as for the pipe problem of §2 since the effect of the nonlinear term in the inner region is $\mathcal{O}(\varepsilon^2)$, which is transcendentally small compared to the logarithmic terms. Hence, we require that W_0 has the following singular behavior as $x \to x_0$ (see equation (3.18)):

$$W_0 = \alpha + \gamma + \gamma\nu \log|x - x_0| + o(1)\,, \quad \text{as} \quad x \to x_0\,. \tag{3.112}$$

Here $\gamma = \gamma(\nu)$ is to be found and ν is defined in terms of the logarithmic capacitance d of (3.15) by $\nu = -1/\log(\varepsilon d)$.

At this stage the asymptotic treatment of the nonlinear problem (3.110) differs slightly from its linear counterpart (3.10). We suppose that for some range of the parameter S we can find a solution to (3.111) with the singular behavior

$$W_0 \sim S \log |x - x_0| \,, \quad \text{as} \quad x \to x_0 \,. \tag{3.113}$$

Then, in terms of this solution we define the regular part $R = R(S; x_0)$ of this Coulomb singularity by

$$R(S; x_0) = \lim_{x \to x_0} \left(W_0 - S \log |x - x_0| \right) \,. \tag{3.114 a}$$

In general R is a nonlinear function of S at each x_0. Therefore, we have

$$W_0 \sim S \log |x - x_0| + R(S; x_0) + o(1) \,, \quad \text{as} \quad x \to x_0 \,. \tag{3.114 b}$$

Equating (3.114 *b*) to (3.112) we get $S = \nu\gamma$ and $R = \alpha + \gamma$, where $\nu = -1/\log(\varepsilon d)$. For fixed εd and α, these relations are two nonlinear algebraic equations for the two unknowns S and γ. Alternatively, we can view these relations as providing a parametric representation of the desired curve $\gamma = \gamma(\nu)$ in the form $\nu = \nu(S)$ and $\gamma = \gamma(S)$, where

$$\gamma = R(S; x_0) - \alpha \,, \qquad \nu = \frac{S}{R(S; x_0) - \alpha} \,. \tag{3.115}$$

The equation for ν in (3.115) is an implicit equation determining S in terms of ε from $\nu = -1/\log(\varepsilon d)$. Therefore, we can analytically sum all of the logarithmic terms in the expansion of the solution to (3.110) provided that we compute the solution to (3.111), with singular behavior (3.113), and then identify $R(S; x_0)$ from (3.114 *a*). In general this must be done numerically. However, we now illustrate the method with an example where $R(S; x_0)$ can be calculated analytically.

Let Ω be the unit disk, and take $b = \infty$, $w_b = 0$, $F(w) = e^w$, and assume that Ω_ε is an arbitrarily-shaped hole centered at the origin. Then, (3.111) and (3.113) reduce to a radially symmetric problem for $W_0(r)$, given by

$$W_0'' + \frac{1}{r} W_0' + e^{W_0} = 0 \,, \quad 0 < r \leq 1 \,; \quad W_0 = 0 \,, \quad \text{on} \quad r = 1 \,, \tag{3.116 a}$$

$$W_0 \sim S \log r \,, \quad \text{as} \quad r \to 0 \,, \tag{3.116 b}$$

where $r = |x|$. This problem (3.116) can be solved analytically by first introducing the new variables v and η defined by

$$v = W_0 - S \log r \,, \qquad \eta = r^{1+S/2} \,. \tag{3.117}$$

When $S > -2$, we then obtain that $v = v(\eta)$ is smooth and satisfies

$$v'' + \frac{1}{\eta} v' + \left(1 + \frac{S}{2} \right)^{-2} e^v = 0 \,, \quad 0 \leq \eta \leq 1 \,; \quad v = 0 \,, \quad \text{on} \quad \eta = 1 \,. \tag{3.118}$$

The well-known solution to (3.118) (see [**77**]) can be written in parametric form as

$$v(\eta) = 2 \log \left(\frac{1 + \rho}{1 + \rho\eta^2} \right) \,, \tag{3.119 a}$$

where $\rho = \rho(S)$ is given by

$$\left(1 + \frac{S}{2} \right)^{-2} = \frac{8\rho}{(1 + \rho)^2} \,. \tag{3.119 b}$$

The maximum of the right-hand side of (3.119 *b*) is 2 and occurs when $\rho = 1$. Therefore, for there to be a solution to (3.116) we require that $(1 + S/2)^2 > 1/2$, which yields that $S > \sqrt{2} - 2$. When $S > \sqrt{2} - 2$, (3.119 *b*) has two roots for ρ, and hence (3.116) has two solutions. Let us consider the solution with the smaller root, which we label by $\rho_-(S)$. Then, we calculate that

$$\rho_-(S) = (S+1)(S+3) - (S+2)\left[(S+2)^2 - 2\right]^{1/2} . \tag{3.120}$$

Setting $\eta = 0$ in (3.119 a), and using (3.117), we compare with (3.114 a) to conclude that $R(S;\mathbf{0}) = v(0)$, which yields

$$R(S;\mathbf{0}) = 2\log(1 + S/2) + \log\left[8\rho_-(S)\right] . \tag{3.121}$$

Substituting (3.121) into (3.115) gives a parametric representation of the curve $\gamma = \gamma(\nu)$ in the form $\nu = \nu(S)$ and $\gamma = \gamma(S)$.

4 Two Specific Applications of Strong Localized Perturbation Theory

In this section we discuss two recent applications, one in 2-D and the other in 3-D, where strong localized perturbation theory has been applied.

4.1 The Persistence Threshold Problem in Mathematical Ecology

The application of strong localized perturbation theory in this subsection is based on [**45**]. The diffusive logistic model, which describes the evolution of a population with density $u(x,t)$ diffusing with constant diffusivity $D = 1/\lambda > 0$ throughout some habitat represented by a bounded domain $\Omega \subset \mathbb{R}^2$, is formulated as

$$u_t = \Delta u + \lambda u\left[m(x) - u\right] , \quad x \in \Omega\,; \qquad \partial_n u = 0\,, \quad x \in \partial\Omega\,; \qquad u(x,0) = u_0(x) \geq 0\,, \qquad x \in \Omega\,. \tag{4.1}$$

The no-flux boundary condition in (4.1) specifies that no individuals cross the boundary of the habitat Ω. The initial population density $u_0(x)$ is non-negative. The function $m(x)$ represents the growth rate for the species, with $m(x) > 0$ in favorable parts of the habitat, and $m(x) < 0$ in unfavorable parts of the habitat. The integral $\int_\Omega m\,dx$ measures the total resources available in the spatially heterogeneous environment. With respect to applications in ecology, this model was first formulated in [**68**].

To determine the stability of the extinction equilibrium solution $u = 0$, we set $u = \phi(x)e^{-\sigma t}$ in (4.1), where $\phi(x) \ll 1$, to obtain that ϕ satisfies

$$\Delta\phi + \lambda m(x)\phi = -\sigma\phi\,, \quad x \in \Omega; \qquad \partial_n\phi = 0\,, \quad x \in \partial\Omega\,. \tag{4.2}$$

The threshold for species persistence is determined by the stability border of the extinct solution $u = 0$. At this bifurcation point, the eigenvalue of the linearized problem about the zero solution must pass through zero. Therefore, by setting $\sigma = 0$ in (4.2) the problem reduces to the determination of a scalar λ and a function ϕ that satisfies the indefinite weight eigenvalue problem

$$\Delta\phi + \lambda m(x)\phi = 0\,, \quad x \in \Omega\,; \qquad \partial_n\phi = 0\,, \quad x \in \partial\Omega\,; \quad \int_\Omega \phi^2\,dx = 1\,. \tag{4.3}$$

We say that $\lambda_1 > 0$ is a positive principal eigenvalue of (4.3) if the corresponding eigenfunction ϕ_1 of (4.3) is positive in Ω. It is well-known (cf. [**7**], [**28**], [**63**]) that (4.3) has a unique positive principal eigenvalue λ_1 if and only if

$\int_\Omega m\,dx < 0$ and the set $\Omega^+ = \{x \in \Omega \; ; \; m(x) > 0\}$ has positive measure. Such an eigenvalue is the smallest positive eigenvalue of (4.3).

The positive principal eigenvalue λ_1 is interpreted as the persistence threshold for the species. It is well-known that if $\lambda < \lambda_1$, then $u(x,t) \to 0$ uniformly in $\bar{\Omega}$ for all non-negative and non-trivial initial data, so that the population tends to extinction. Alternatively, if $\lambda > \lambda_1$, then $u(x,t) \to u^*(x)$ uniformly in $\bar{\Omega}$ as $t \to \infty$, where u^* is the unique positive steady-state solution of (4.1). For this range of λ the species will persist. Many mathematical results for (4.1) under different boundary conditions are given in the pioneering works of [**8**], [**9**], and [**10**]. Related results for multi-species interactions and other mathematical problems in ecology are given in [**11**] (see also the survey article of [**48**]).

An interesting problem in mathematical ecology is to determine, among all functions $m(x)$ for which a persistence threshold exists, which $m(x)$ yields the smallest λ_1 for a fixed amount of total resources $\int_\Omega m\,dx$. In other words, we seek to determine the optimum arrangement of favorable habitats in Ω in order to allow the species to persist for the largest possible diffusivity D. This optimization problem was originally posed and studied in [**8**] and [**10**]. For (4.1) under Neumann boundary conditions in a two-dimensional domain Ω, it was proved in Theorem 1.1 of [**47**] that the optimum $m(x)$ is piecewise continuous and of bang-bang type. An earlier result showing the existence of a similar bang-bang optimal control for $m(x)$ for the Dirichlet problem was given in [**8**]. For (4.1) posed in a one-dimensional interval $0 < x < 1$, it was proved in Theorem 1.2 of [**47**] that the optimal $m(x)$ consists of a single favorable habitat attached to one of the two endpoints of the interval. Related results were given in [**10**] under Dirichlet, Neumann, or Robin type boundary conditions.

In this subsection, we asymptotically calculate, and then optimize, the persistence threshold λ_1 for a particular class of piecewise constant growth rate function $m = m_\varepsilon(x)$ in an arbitrary two-dimensional domain. We assume that $m_\varepsilon(x)$ is localized to n small circular patches of radii $\mathcal{O}(\varepsilon)$, each of which is centered either inside Ω or on $\partial\Omega$. We assume that the boundary $\partial\Omega$ is piecewise differentiable, but allow for the domain boundary to have a finite numbers of corners, each with a non-zero contact angle, which arises from a jump discontinuity of the slope of the tangent line to the boundary. We denote $\Omega^I \equiv \{x_1, \ldots, x_n\} \cap \Omega$ to be the set of the centers of the interior patches, while $\Omega^B \equiv \{x_1, \ldots, x_n\} \cap \partial\Omega$ is the set of the centers of the boundary patches. We assume that the patches are well-separated in the sense that $|x_i - x_j| \gg \mathcal{O}(\varepsilon)$ for $i \neq j$ and that the interior patches are not too close to the boundary, i.e. $\text{dist}(x_j, \partial\Omega) \gg \mathcal{O}(\varepsilon)$ whenever $x_j \in \Omega^I$. To accommodate a boundary patch, we will associate with each x_j for $j = 1, \ldots, n$, an angle $\pi\alpha_j$ representing the angular fraction of a circular patch that is contained within Ω. More specifically, $\alpha_j = 2$ whenever $x_j = \Omega^I$, $\alpha_j = 1$ when $x_j \in \Omega^B$ and x_j is a point where $\partial\Omega$ is smooth, and $\alpha_j = 1/2$ when $x_j \in \partial\Omega$ is at a corner point of $\partial\Omega$ for which the two (one-sided) tangent lines to the boundary intersect at a $\pi/2$ contact angle (see Fig. 6). The growth rate function $m = m_\varepsilon(x)$ in (4.3) is taken to have the specific form

$$m = m_\varepsilon(x) \equiv \begin{cases} m_j/\varepsilon^2 \,, & x \in \Omega_{\varepsilon_j} \,, \quad j = 1, \ldots, n \,, \\ -m_b \,, & x \in \Omega \backslash \bigcup_{j=1}^n \Omega_{\varepsilon_j} \,. \end{cases} \tag{4.4}$$

Here $\Omega_{\varepsilon_j} \equiv \{x \,|\, |x - x_j| \le \varepsilon\rho_j \cap \Omega\}$, so that each patch Ω_{ε_j} is the portion of a circular disk of radius $\varepsilon\rho_j$ that is strictly inside Ω. The constant m_j is the local growth rate of the j^{th} patch, with $m_j > 0$ for a favorable habitat and $m_j < 0$ for an unfavorable habitat. The constant $m_b > 0$ is the background bulk decay rate for the unfavorable habitat. In terms of this growth rate function, the condition of [**7**], [**28**], and [**63**] for the existence of a persistence threshold is that one of the m_j for $j = 1, \ldots, n$ must be positive, and that the following asymptotically valid inequality on the total resources hold as $\varepsilon \to 0$:

$$\int_\Omega m_\varepsilon \, dx = -m_b|\Omega| + \frac{\pi}{2}\sum_{j=1}^{n} \alpha_j m_j \rho_j^2 + \mathcal{O}(\varepsilon^2) < 0 \,. \tag{4.5}$$

Here $|\Omega|$ denotes the area of Ω. We assume that the parameters are chosen so that (4.5) is satisfied. A schematic plot of a domain with interior circular patches, and with portions of circular patches on its boundary, is shown in Fig. 6.

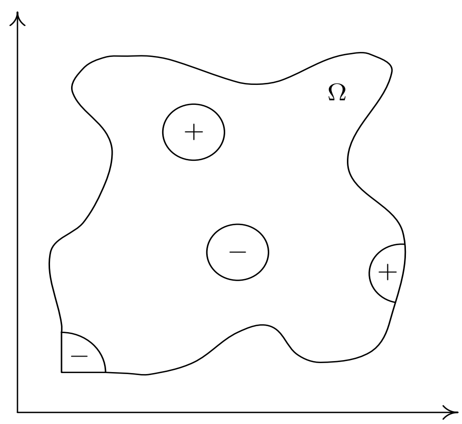


FIGURE 6. Schematic plot of a two-dimensional domain Ω with localized strongly favorable $(+)$ or unfavorable $(-)$ habitats, or patches, as described by (4.4). The patches inside the domain are small circular disks. On the domain boundary, the patches are the portions of circular disks that lie within the domain. The unfavorable boundary habitat in the lower left part of this figure is at a $\pi/2$ corner of $\partial\Omega$.

This specific form for $m_\varepsilon(x)$ is motivated by Theorem 1.1 of [**47**] that states that the optimal growth rate function must be of bang-bang type, and the result of [**59**] that shows that a sufficiently small optimum favorable habitat must be a circular disk.

We first consider the case of one interior circular patch centered at $x_0 \in \Omega$, with $\text{dist}(x_0, \partial\Omega) \gg \mathcal{O}(\varepsilon)$. We asymptotically calculate the positive principal eigenvalue $\lambda > 0$ and corresponding eigenfunction $\phi > 0$ of

$$\Delta\phi + \lambda\, m_\varepsilon(x)\phi = 0\,, \quad x \in \Omega; \qquad \partial_n\phi = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega \phi^2\, dx = 1\,, \tag{4.6 a}$$

in the small patch radius limit $\varepsilon \to 0$, where the growth rate function $m_\varepsilon(x)$ is defined as

$$m_\varepsilon(x) = \begin{cases} m_+/\varepsilon^2\,, & x \in \Omega_{\varepsilon_0}\,, \\ -m_b, & x \in \Omega\backslash\Omega_{\varepsilon_0}\,. \end{cases} \tag{4.6 b}$$

Here the patch Ω_{ε_0} is the circular disk $\Omega_{\varepsilon_0} \equiv \{x \,|\, |x - x_0| \le \varepsilon\}$. In (4.6 b), $m_+ > 0$ is the local growth rate of the favorable habitat, while $m_b > 0$ gives the background bulk decay rate for the unfavorable habitat.

The condition $\int_\Omega m\, dx < 0$ for the existence of a positive principal eigenvalue is asymptotically equivalent to

$$\int_\Omega m\, dx = -m_b|\Omega| + \pi m_+ + \mathcal{O}(\varepsilon^2) < 0\,, \tag{4.7}$$

in the limit $\varepsilon \to 0$. We assume that m_b and m_+ are chosen so that this condition holds.

We expand the positive principal eigenvalue λ of (4.6) as

$$\lambda \sim \mu_0\nu + \mu_1\nu^2 + \cdots\,, \qquad \nu = -1/\log\varepsilon\,, \tag{4.8}$$

for some coefficients μ_0 and μ_1 to be found. In the outer region, defined away from an $\mathcal{O}(\varepsilon)$ neighborhood of x_0, we expand the corresponding eigenfunction as

$$\phi \sim \phi_0 + \nu\phi_1 + \nu^2\phi_2 + \cdots\,. \tag{4.9}$$

Upon substituting (4.8) and (4.9) into (4.6), we obtain that ϕ_0 is a constant. The normalization condition $\int_\Omega \phi_0^2\, dx = 1$ yields $\phi_0 = |\Omega|^{-1/2}$, where $|\Omega|$ is the area of Ω. In addition, we obtain that ϕ_1 and ϕ_2 satisfy

$$\Delta\phi_1 = \mu_0 m_b\phi_0\,, \quad x \in \Omega\backslash\{x_0\}\,; \qquad \partial_n\phi_1 = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega \phi_1\, dx = 0\,, \tag{4.10 a}$$

$$\Delta\phi_2 = \mu_1 m_b\phi_0 + \mu_0 m_b\phi_1\,, \quad x \in \Omega\backslash\{x_0\}\,; \qquad \partial_n\phi_2 = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega \left(\phi_1^2 + 2\phi_0\phi_2\right)\, dx = 0\,. \tag{4.10 b}$$

The matching of ϕ_1 and ϕ_2 to an inner solution defined in an $\mathcal{O}(\varepsilon)$ neighborhood of the patch at x_0, as done below, will yield singularity conditions for ϕ_1 and ϕ_2 as $x \to x_0$.

In the inner region near the patch centered at x_0 we introduce the local variables y and ψ by

$$y = \varepsilon^{-1}(x - x_0)\,, \qquad \psi(y) = \phi(x_0 + \varepsilon y)\,. \tag{4.11}$$

Then, (4.6) becomes

$$\Delta\psi = \begin{cases} -\lambda m_+\psi\,, & |y| < 1\,, \\ \mathcal{O}(\varepsilon^2)\,, & |y| > 1\,. \end{cases} \tag{4.12}$$

We then represent the inner approximation to the eigenfunction as

$$\psi \sim \psi_0 + \nu\psi_1 + \nu^2\psi_2 + \cdots\,, \qquad \nu = -1/\log\varepsilon\,. \tag{4.13}$$

We substitute (4.13) and (4.8) into (4.12), and collect powers of ν, to obtain that ψ_0 is an unknown constant, and that ψ_1 and ψ_2 satisfy

$$\Delta\psi_k = \begin{cases} \mathcal{F}_k\,, & |y| \le 1\,, \\ 0\,, & |y| \ge 1\,. \end{cases} \tag{4.14 a}$$

Here $\mathcal{F}_k$ for $k = 1, 2$ is defined by

$$\mathcal{F}_1 = -\mu_0 m_+\psi_0\,, \qquad \mathcal{F}_2 = -\mu_0 m_+\psi_1 - \mu_1 m_+\psi_0\,. \tag{4.14 b}$$

We then calculate the solution ψ_1 to (4.14) as

$$\psi_1 = \begin{cases} A_1\rho^2/2 + \bar{\psi}_1\,, & \rho \leq 1\,, \\ A_1 \log\rho + \frac{A_1}{2} + \bar{\psi}_1\,, & \rho \geq 1\,, \end{cases} \tag{4.15 a}$$

where $\rho = |y|$. Here $\bar{\psi}_1$ is an unknown constant, and A_1 is given by

$$A_1 = \frac{\mathcal{F}_1}{2} = -\frac{1}{2}\mu_0 m_+ \psi_0\,. \tag{4.15 b}$$

In addition, for the solution ψ_2 to (4.14) we calculate its far-field behavior as

$$\psi_2 \sim A_2 \log\rho + \mathcal{O}(1)\,, \quad \text{as} \quad \rho \to \infty\,, \qquad A_2 \equiv \int_0^1 \mathcal{F}_2\,\rho\,d\rho\,. \tag{4.16 a}$$

We then calculate A_2 by using (4.15) and (4.14 b) for $\mathcal{F}_2$ to get

$$A_2 = -\mu_0 m_+ \int_0^1 \left(A_1\frac{\rho^2}{2} + \bar{\psi}_1\right)\rho\,d\rho - \frac{1}{2}\mu_1 m_+ \psi_0 = \frac{A_1}{\psi_0}\left(\frac{A_1}{4} + \bar{\psi}_1 + \frac{\mu_1}{\mu_0}\psi_0\right)\,. \tag{4.16 b}$$

The matching condition is that the near-field behavior as $x \to x_0$ of the outer representation of the eigenfunction must agree asymptotically with the far-field behavior of the inner eigenfunction as $|y| = \varepsilon^{-1}|x - x_0| \to \infty$, so that

$$\phi_0 + \nu\phi_1 + \nu^2\phi_2 + \cdots \sim \psi_0 + \nu\psi_1 + \nu^2\psi_2 + \cdots\,. \tag{4.17}$$

Upon using the far-field behavior of ψ_1 and ψ_2, as given in (4.15) and (4.16) respectively, we obtain that (4.17) becomes

$$\phi_0 + \nu\phi_1 + \nu^2\phi_2 + \cdots \sim \psi_0 + A_1 + \nu\left(A_1\log|x - x_0| + \frac{A_1}{2} + \bar{\psi}_1 + A_2\right) + \nu^2\left(A_2\log|x - x_0| + \mathcal{O}(1)\right)\,. \tag{4.18}$$

Since ϕ_0 and ψ_0 are constants, we obtain the first matching condition that

$$\phi_0 = \psi_0 + A_1\,. \tag{4.19}$$

Then, from the $\mathcal{O}(\nu)$ terms in the matching condition (4.18), we obtain that ϕ_1 satisfies (4.10 a) subject to the singularity behavior

$$\phi_1 \sim A_1\log|x - x_0| + \frac{A_1}{2} + \bar{\psi}_1 + A_2\,, \quad \text{as} \quad x \to x_0\,. \tag{4.20}$$

We remark that the singularity behavior in (4.20) specifies both the regular and singular part of a Coulomb singularity. Consequently, this singularity structure provides one constraint relating A_1, A_2, and $\bar{\psi}_1$.

The problem for ϕ_1 can be written in terms of the Dirac distribution as

$$\Delta\phi_1 = \mu_0 m_b \phi_0 + 2\pi A_1 \delta(x - x_0)\,, \quad x \in \Omega\,; \qquad \partial_n\phi_1 = 0\,, \quad x \in \partial\Omega\,. \tag{4.21}$$

The divergence theorem then yields

$$A_1 = -\frac{1}{2\pi}\left(\mu_0 m_b |\Omega| \phi_0\right)\,. \tag{4.22}$$

Next, we write the solution to (4.21) in terms of the Neumann Green's function $G(x; x_0)$ as

$$\phi_1 = -2\pi A_1 G(x; x_0) = \mu_0 m_b |\Omega| \phi_0 G(x; x_0)\,. \tag{4.23}$$

Here $G(x;x_0)$ is the unique solution to

$$\Delta G = \frac{1}{|\Omega|} - \delta(x-x_0)\,, \quad x\in\Omega\,; \qquad \partial_n G = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega G\,dx = 0\,, \tag{4.24 a}$$

$$G(x;x_0) \sim -\frac{1}{2\pi}\log|x-x_0| + R(x_0;x_0)\,, \quad \text{as} \quad x\to x_0\,, \tag{4.24 b}$$

where $R(x_0;x_0)$ is the regular part of $G(x;x_0)$ at $x=x_0$. By expanding ϕ_1 in (4.23) as $x\to x_0$ and equating the non-singular part of the resulting expression with that of (4.20), we obtain

$$-2\pi A_1 R(x_0;x_0) = \frac{A_1}{2} + \bar{\psi}_1 + A_2\,. \tag{4.25}$$

Finally, we obtain from the $\mathcal{O}(\nu^2)$ terms in the matching condition (4.18) that $\phi_2 \sim A_2\log|x-x_0|$ as $x\to x_0$, where ϕ_2 is the solution to (4.10 *b*). In terms of the Dirac mass, this problem for ϕ_2 can be written as

$$\Delta\phi_2 = \mu_1 m_b\phi_0 + \mu_0 m_b \phi_1 + 2\pi A_2\delta(x-x_0)\,, \quad x\in\Omega\,; \qquad \partial_n\phi_2 = 0\,, \quad x\in\partial\Omega\,, \tag{4.26}$$

with normalization condition $\int_\Omega \left(\phi_1^2 + 2\phi_0\phi_2\right)\,dx = 0$. The divergence theorem, together with $\int_\Omega \phi_1\,dx = 0$, then yields that

$$2\pi A_2 = -\mu_1 m_b|\Omega|\phi_0\,. \tag{4.27}$$

The leading-order eigenvalue correction μ_0 is obtained by combining (4.19) and (4.22), together with using $A_1 = -\mu_0 m_+\psi_0/2$ from (4.15 *b*). This yields that

$$\phi_0 = \frac{\pi m_+}{|\Omega| m_b}\psi_0\,, \qquad \phi_0 = \left(1 - \frac{\mu_0 m_+}{2}\right)\psi_0\,. \tag{4.28}$$

Therefore, since $\phi_0 = |\Omega|^{-1/2}$, we obtain

$$\mu_0 = \frac{2}{m_+}\left[1 - \frac{\pi m_+}{|\Omega| m_b}\right]\,, \qquad \psi_0 = \frac{|\Omega| m_b}{\pi m_+}\phi_0\,, \qquad \phi_0 = |\Omega|^{-1/2}\,. \tag{4.29}$$

Since $\int_\Omega m\,dx < 0$, then $m_+\pi/(|\Omega|m_b) < 1$ from (4.7). Consequently, it follows from (4.29) that $\mu_0 > 0$. Next, we combine (4.22) and (4.27) to evaluate the ratio A_2/A_1 as $A_2/A_1 = \mu_1/\mu_0$. Upon using $A_2/A_1 = \mu_1/\mu_0$ in (4.25) and (4.16 *b*), we readily determine $\bar{\psi}_1$ and the eigenvalue correction μ_1 as

$$\bar{\psi}_1 = -\frac{A_1}{4}\,, \qquad \mu_1 = -\left(\frac{1}{4} + 2\pi R(x_0;x_0)\right)\mu_0\,. \tag{4.30}$$

Finally, a two-term expansion for the eigenfunction in the outer region is obtained from (4.9) by using (4.23) for ϕ_1. The corresponding two-term inner approximation to the eigenfunction is given by (4.13), where ψ_1 is given in (4.15) with $\bar{\psi}_1 = -A_1/4$. We summarize our result as follows:

Principal Result 4.1: *In the limit of small patch radius, $\varepsilon\to 0$, the positive principal eigenvalue λ of (4.6) has the following two-term asymptotic expansion in terms of the logarithmic gauge function $\nu = -1/\log\varepsilon$:*

$$\lambda = \mu_0\nu - \mu_0\nu^2\left[\frac{1}{4} + 2\pi R(x_0;x_0)\right] + \mathcal{O}(\nu^3)\,; \qquad \mu_0 \equiv \frac{2}{m_+}\left[1 - \frac{\pi m_+}{|\Omega| m_b}\right]\,. \tag{4.31 a}$$

A two-term asymptotic expansion for the corresponding eigenfunction in the outer region $|x-x_0| \gg \mathcal{O}(\varepsilon)$ is

$$\phi \sim \phi_0\left(1 + \nu\mu_0 m_b|\Omega| G(x;x_0)\right)\,. \tag{4.31 b}$$

Here $G(x;x_0)$ is the Neumann Green's function of (4.24) with regular part $R(x_0;x_0)$. The corresponding inner approximation to the eigenfunction, with $y = \varepsilon^{-1}(x - x_0)$ and $\rho = |y| = \mathcal{O}(1)$, is

$$\psi \sim \frac{m_b|\Omega|}{m_+\pi}\phi_0\left(1 - \frac{\mu_0 m_+}{2}\nu\tilde{\psi}_1(\rho)\right), \tag{4.31 c}$$

where $\phi_0 = |\Omega|^{-1/2}$, and $\tilde{\psi}_1(\rho)$ is defined by

$$\tilde{\psi}_1(\rho) \equiv \begin{cases} \rho^2/2 - 1/4\,, & \rho \le 1\,, \\ \log\rho + 1/4\,, & \rho \ge 1\,. \end{cases} \tag{4.31 d}$$

Next, we let the center x_0 of the circular patch be on $\partial\Omega$. We assume that $\partial\Omega$ is piecewise differentiable, but allow for $\partial\Omega$ to have corners with nonzero contact angle. The boundary patch $\Omega_{\varepsilon_0} \equiv \{x \,|\, |x - x_0| \le \varepsilon\rho_0 \cap \Omega\}$ with $x_0 \in \partial\Omega$ is the portion of a circular disk of radius $\varepsilon\rho_0$ that is strictly contained within Ω. Here $\rho_0 = \mathcal{O}(1)$ is introduced in order to construct a boundary patch that has the same area as an interior patch.

In the limit $\varepsilon \to 0$, and for $x - x_0 = \mathcal{O}(\varepsilon)$, we define $\pi\alpha_0$ to be angular fraction of the circular patch that is contained within Ω. More specifically, $\alpha_0 = 1$ whenever x_0 is at a smooth point of $\partial\Omega$, and $\alpha_0 = 1/2$ when x_0 is at a $\pi/2$ corner of $\partial\Omega$. The eigenvalue problem associated with this boundary patch is

$$\Delta\phi + \lambda\, m_\varepsilon(x)\phi = 0\,, \quad x \in \Omega; \qquad \partial_n\phi = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega \phi^2\, dx = 1\,, \tag{4.32 a}$$

where $m_\varepsilon(x)$ is defined as

$$m_\varepsilon(x) = \begin{cases} m_+/\varepsilon^2\,, & x \in \Omega_{\varepsilon_0}\,, \\ -m_b\,, & x \in \Omega\backslash\Omega_{\varepsilon_0}\,. \end{cases} \tag{4.32 b}$$

The condition $\int_\Omega m\, dx < 0$ is asymptotically equivalent when $\varepsilon \to 0$ to

$$\int_\Omega m\, dx = -m_b|\Omega| + \frac{\alpha_0\pi}{2}\left(m_+\rho_0^2\right) + \mathcal{O}(\varepsilon^2) < 0\,. \tag{4.33}$$

We assume that this condition on $\int_\Omega m\, dx$ holds. Since the asymptotic calculation of λ for a boundary patch is similar to that for the interior patch case, we mainly highlight the new features that are required in the analysis.

We first expand λ as in (4.8) in terms of $\nu = -1/\log\varepsilon$. In the outer region, defined for $|x - x_0| \gg \mathcal{O}(\varepsilon)$, we expand the outer solution as in (4.9) to obtain that ϕ_0 is a constant, and that ϕ_1 and ϕ_2 satisfy (4.10 a) and (4.10 b) in Ω, respectively, with $\partial_n\phi_k = 0$ for $x \in \partial\Omega\backslash\{x_0\}$ for $k = 1, 2$.

Since the expansion of the inner solution is again in powers of $\nu = -1/\log\varepsilon$ as in (4.13), we can neglect to any power of ν the effect of the curvature of the domain boundary near $x = x_0$, provided that this curvature is finite. Consequently, when x_0 is at a smooth point of $\partial\Omega$, we can approximate $\partial\Omega$ near $x = x_0$ by the tangent line to $\partial\Omega$ through $x = x_0$. Alternatively, when x_0 is at corner point of $\partial\Omega$, the inner region is the angular wedge of angle $\pi\alpha_0$ bounded by the intersection of the one-sided tangent lines to $\partial\Omega$ at $x = x_0$. We then introduce the inner variable $y = \varepsilon^{-1}(x - x_0)$ so that the inner region is the angular wedge $\beta_0 < \arg y \le \alpha_0\pi + \beta_0$ for some β_0. The favorable habitat is the circular patch $|y| \le \rho_0$ that lies within this wedge. Since the no-flux boundary conditions $\partial_n\psi = 0$ holds on the two sides of the wedge, we look for a local radially symmetric inner solution within the angular wedge.

Therefore, in the inner region, we expand the inner solution as in (4.13) and obtain that ψ_0 is a constant, and that ψ_k for $k = 1, 2$ satisfies

$$\Delta \psi_k = \begin{cases} \mathcal{F}_k \,, & |y| \leq \rho_0 \,, \quad \beta_0 \leq \arg y \leq \pi\alpha_0 + \beta_0 \,, \\ 0 \,, & |y| \geq \rho_0 \,, \quad \beta_0 \leq \arg y \leq \pi\alpha_0 + \beta_0 \,. \end{cases} \tag{4.34}$$

Here $\mathcal{F}_k$ for $k = 1, 2$ are defined in (4.14 b). The solution for ψ_1, with $\rho = |y|$, is

$$\psi_1 = \begin{cases} A_1 \left(\frac{\rho^2}{2\rho_0^2} \right) + \bar{\psi}_1 \,, & 0 \leq \rho \leq \rho_0 \,, \quad \beta_0 \leq \arg y \leq \pi\alpha_0 + \beta_0 \,, \\ A_1 \log \left(\frac{\rho}{\rho_0} \right) + \frac{A_1}{2} + \bar{\psi}_1 \,, & \rho \geq \rho_0 \,, \quad \beta_0 \leq \arg y \leq \pi\alpha_0 + \beta_0 \,, \end{cases} \tag{4.35}$$

where $\bar{\psi}_1$ is an unknown constant and $A_1 = \mathcal{F}_1 \rho_0^2/2$. For ψ_2, we obtain that $\psi_2 \sim A_2 \log \rho$ as $\rho \to \infty$. The calculation of A_2 proceeds exactly as in (4.16 b) to obtain

$$A_1 = -\frac{\mu_0}{2} m_+ \rho_0^2 \psi_0 \,, \qquad A_2 = \frac{A_1}{\psi_0} \left(\frac{A_1}{4} + \bar{\psi}_1 + \frac{\mu_1}{\mu_0} \psi_0 \right) . \tag{4.36}$$

The matching condition between the outer solution as $x \to x_0$ and the inner solution for $|y| = \varepsilon^{-1}|x - x_0| \to \infty$ is given by (4.17). Upon using (4.35) for ψ_1 when $\rho \gg 1$, together with $\psi_2 \sim A_2 \log \rho$ for $\rho \gg 1$, we obtain that (4.17) becomes

$$\phi_0 + \nu\phi_1 + \nu^2\phi_2 + \cdots \sim \psi_0 + A_1 + \nu \left(A_1 \log|x - x_0| - A_1 \log \rho_0 + \frac{A_1}{2} + \bar{\psi}_1 + A_2 \right) + \nu^2 \left(A_2 \log|x - x_0| + \mathcal{O}(1) \right) . \tag{4.37}$$

The leading order matching condition from (4.37) is that

$$\phi_0 = \psi_0 + A_1 \,. \tag{4.38}$$

From the $\mathcal{O}(\nu)$ terms in (4.37) and (4.10 a), we obtain that ϕ_1 satisfies

$$\Delta \phi_1 = \mu_0 m_b \phi_0 \,, \quad x \in \Omega \,; \qquad \partial_n \phi_1 = 0 \,, \quad x \in \partial\Omega \backslash \{x_0\} \,; \qquad \int_\Omega \phi_1 \, dx = 0 \,, \tag{4.39 a}$$

$$\phi_1 \sim A_1 \log|x - x_0| - A_1 \log \rho_0 + \frac{A_1}{2} + \bar{\psi}_1 + A_2 \,, \quad \text{as} \quad x \to x_0 \,. \tag{4.39 b}$$

Moreover, from the $\mathcal{O}(\nu^2)$ terms in (4.37) and the problem for ϕ_2 (4.10 b), we get that ϕ_2 satisfies

$$\Delta \phi_2 = \mu_1 m_b \phi_0 + \mu_0 m_b \phi_1 \,, \quad x \in \Omega \,; \qquad \partial_n \phi_2 = 0 \,, \quad x \in \partial\Omega \backslash \{x_0\} \,; \qquad \int_\Omega \left(\phi_1^2 + 2\phi_0\phi_2 \right) \, dx = 0 \,. \tag{4.40 a}$$

$$\phi_2 \sim A_2 \log|x - x_0| + \mathcal{O}(1) \,, \quad \text{as} \quad x \to x_0 \,. \tag{4.40 b}$$

Next, we apply the divergence theorem to (4.39) over $\Omega \backslash \Omega_\sigma$, where Ω_σ is a wedge of angle $\pi\alpha_0$ and small radius $\sigma \ll 1$ centered at $x_0 \in \partial\Omega$. Imposing the singularity condition (4.39 b) on $|x - x_0| = \sigma$ and taking the limit $\sigma \to 0$, we readily derive that

$$\mu_0 m_b |\Omega| \phi_0 = -\alpha_0 \pi A_1 \,. \tag{4.41}$$

In a similar way, the divergence theorem applied to (4.40), and noting that $\int_\Omega \phi_1 \, dx = 0$, determines A_2 as

$$\mu_1 m_b |\Omega| \phi_0 = -\alpha_0 \pi A_2 \,. \tag{4.42}$$

Therefore, we conclude from (4.41) and (4.42) that $A_2/A_1 = \mu_1/\mu_0$, which yields $\bar{\psi}_1 = -A_1/4$ from the equation for A_2 in (4.36). Then, by combining (4.38), (4.36) for A_1, and (4.41), we readily obtain that

$$\psi_0 = \frac{2m_b|\Omega|}{\alpha_0\pi m_+\rho_0^2}\phi_0 \,, \qquad \mu_0 = \frac{2}{m_+\rho_0^2}\left[1 - \frac{\alpha_0\pi m_+\rho_0^2}{2m_b|\Omega|}\right] . \tag{4.43}$$

Since $\int_\Omega m\, dx < 0$ from (4.33), it follows that $\mu_0 > 0$ in (4.43).

To solve (4.39), we introduce the surface Neumann Green's function $G_s(x;x_0)$, defined as the unique solution of

$$\Delta G_s = \frac{1}{|\Omega|}\,, \quad x \in \Omega\,; \qquad \partial_n G_s = 0\,, \qquad x \in \partial\Omega\backslash\{x_0\}\,; \qquad \int_\Omega G_s\, dx = 0\,, \tag{4.44 a}$$

$$G_s(x;x_0) \sim -\frac{1}{\alpha_0\pi}\log|x-x_0| + R_s(x_0;x_0)\,, \quad \text{as } x \to x_0 \in \partial\Omega\,. \tag{4.44 b}$$

Here $|\Omega|$ is the area of Ω, and $R_s(x_0;x_0)$ is the regular part of the surface Neumann Green's function at $x = x_0$. Then, the solution to (4.39) is

$$\phi_1 = -\alpha_0\pi A_1 G_s(x;x_0)\,. \tag{4.45}$$

By expanding ϕ_1 as $x \to x_0$ using (4.44 b), we equate the resulting nonsingular part of ϕ_1 as $x \to x_0$ with that in (4.39 b) to obtain

$$-\alpha_0\pi A_1 R_s(x_0;x_0) = -A_1\log\rho_0 + \frac{A_1}{2} + \bar{\psi}_1 + A_2\,. \tag{4.46}$$

We then substitute $\bar{\psi}_1 = -A_1/4$ and $A_2/A_1 = \mu_1/\mu_0$ into (4.46), and solve for μ_1 to get

$$\mu_1 = \mu_0\left[\log\rho_0 - \frac{1}{4} - \alpha_0\pi R_s(x_0;x_0)\right] . \tag{4.47}$$

We summarize our result as follows:

Principal Result 4.2: *In the limit of small boundary patch radius, $\varepsilon \to 0$, a two-term asymptotic expansion for the positive principal eigenvalue λ of (4.32) in terms of $\nu = -1/\log\varepsilon$ is*

$$\lambda = \mu_0\nu - \mu_0\nu^2\left[\frac{1}{4} + \alpha_0\pi R_s(x_0;x_0) - \log\rho_0\right] + \mathcal{O}(\nu^3)\,; \qquad \mu_0 \equiv \frac{2}{m_+\rho_0^2}\left[1 - \frac{\alpha_0\pi m_+\rho_0^2}{2|\Omega|m_b}\right] . \tag{4.48 a}$$

A two-term asymptotic expansion for the corresponding eigenfunction in the outer region $|x-x_0| \gg \mathcal{O}(\varepsilon)$ is

$$\phi \sim \phi_0\left(1 + \nu\mu_0 m_b|\Omega|G_s(x;x_0)\right) . \tag{4.48 b}$$

Here $G_s(x;x_0)$ is the surface Neumann Green's function of (4.44) with regular part $R_s(x_0;x_0)$.

Next, we generalize the analysis above to treat the case of an arbitrary but fixed number n of circular patches, each of which is centered either inside Ω or on $\partial\Omega$. To this end, we asymptotically calculate the positive principal eigenvalue of

$$\Delta\phi + \lambda\, m_\varepsilon(x)\phi = 0\,, \quad x \in \Omega; \qquad \partial_n\phi = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega \phi^2\, dx = 1\,, \tag{4.49 a}$$

where the growth rate function $m_\varepsilon(x)$ is defined by

$$m_\varepsilon(x) = \begin{cases} m_j/\varepsilon^2\,, & x \in \Omega_{\varepsilon_j}\,, \quad j = 1,\ldots,n\,, \\ -m_b\,, & x \in \Omega\backslash\bigcup_{j=1}^n \Omega_{\varepsilon_j}\,. \end{cases} \tag{4.49 b}$$

Here $\Omega_{\varepsilon_j} \equiv \{x \,|\, |x-x_j| \le \varepsilon\rho_j \cap \Omega\}$, so that the patches Ω_{ε_j} are the portions of the circular disks of radius $\varepsilon\rho_j$ that are strictly inside Ω. The constant m_j is the local growth rate of the j^{th} patch, with $m_j > 0$ for a favorable habitat and $m_j < 0$ for an unfavorable habitat. The constant $m_b > 0$ is the background bulk decay rate for the unfavorable habitat. In terms of this patch arrangement, the condition $\int_\Omega m\,dx < 0$ is asymptotically equivalent for $\varepsilon \to 0$ to

$$\int_\Omega m\,dx = -m_b|\Omega| + \frac{\pi}{2}\sum_{j=1}^{n} \alpha_j m_j \rho_j^2 + \mathcal{O}(\varepsilon^2) < 0\,. \tag{4.50}$$

We assume that the parameters are chosen so that this condition holds. The parameters in the growth rate are the centers $x_1, \ldots, x_n$ of the circular patches, their radii $\varepsilon\rho_1, \ldots, \varepsilon\rho_n$, the local growth rates $m_1, \ldots, m_n$, the angular fractions $\pi\alpha_1, \ldots, \pi\alpha_n$ of the circular patches that are contained in Ω, and the constant bulk growth rate m_b. Recall that $\alpha_j = 2$ whenever $x_j \in \Omega$, $\alpha_j = 1$ when $x_j \in \partial\Omega$ and x_j is a point where $\partial\Omega$ is smooth, and $\alpha_j = 1/2$ when $x_j \in \partial\Omega$ is at a $\pi/2$ corner of $\partial\Omega$, etc.

To asymptotically analyze (4.49) we must incorporate both the Neumann Green's function and the surface Neumann Green's function. As such, we define a generalized modified Green's function $G_m(x; x_j)$ by

$$G_m(x; x_j) \equiv \begin{cases} G(x; x_j)\,, & x_j \in \Omega\,, \\ G_s(x; x_j)\,, & x_j \in \partial\Omega\,. \end{cases} \tag{4.51 a}$$

Here $G(x; x_j)$ is the Neumann Green's function of (4.24), and $G_s(x; x_j)$ is the surface Neumann Green's function of (4.44). Therefore, the local behavior of $G_m(x; x_j)$ is

$$G_m(x; x_j) \sim -\frac{1}{\alpha_j \pi}\log|x - x_j| + R_m(x_j; x_j)\,, \quad \text{as} \quad x \to x_j\,, \qquad R_m(x_j; x_j) \equiv \begin{cases} R(x_j; x_j)\,, & x_j \in \Omega\,, \\ R_s(x_j; x_j)\,, & x_j \in \partial\Omega\,. \end{cases} \tag{4.51 b}$$

Here $R(x_j; x_j)$ and $R_s(x_j; x_j)$ are the regular part of the Neumann Green's function (4.24) and the surface Neumann Green's function (4.44), respectively.

For the multiple patch case, the following main result was obtained in §3 of [**45**].

Principal Result 4.3: *In the limit of small patch radius, $\varepsilon \to 0$, the positive principal eigenvalue λ of (4.49) has the following two-term asymptotic expansion in terms of the logarithmic gauge function $\nu = -1/\log\varepsilon$:*

$$\lambda = \mu_0\nu - \mu_0\nu^2\left(\frac{\kappa^t\left(\pi\mathcal{G}_m - \mathcal{P}\right)\kappa}{\kappa^t\kappa} + \frac{1}{4}\right) + \mathcal{O}(\nu^3)\,. \tag{4.52}$$

Here $\mu_0 > 0$ is the first positive root of $\mathcal{B}(\mu_0) = 0$, where $\mathcal{B}(\mu_0)$ is defined by

$$\mathcal{B}(\mu_0) \equiv -m_b|\Omega| + \pi\sum_{j=1}^{n} \frac{\alpha_j m_j \rho_j^2}{2 - m_j\rho_j^2\mu_0}\,. \tag{4.53}$$

In (4.52), $\kappa = (\kappa_1, \ldots, \kappa_n)^t$, where κ_j is defined by

$$\kappa_j \equiv \frac{\sqrt{\alpha_j}\, m_j \rho_j^2}{2 - m_j\rho_j^2\mu_0}\,, \tag{4.54}$$

while $\mathcal{G}_m$ and $\mathcal{P}$ are the $n \times n$ matrices as defined by

$$\mathcal{G}_{mij} = \sqrt{\alpha_i\alpha_j}\,G_{mij}\,, \quad i \neq j\,; \qquad \mathcal{G}_{mjj} = \alpha_j R_{mjj}\,; \qquad \mathcal{P}_{ij} = 0\,, \quad i \neq j\,; \qquad \mathcal{P}_{jj} = \log\rho_j\,. \tag{4.55}$$

In addition, a two-term expansion for the outer solution is given by

$$\phi \sim \phi_0 \left(1 + \nu \pi \mu_0 \sum_{j=1}^{n} \sqrt{\alpha_j} \kappa_j G_m(x; x_j) \right) . \tag{4.56}$$

Problem 4.1: *Give the derivation of equation (4.53) for the leading-order coefficient μ_0 in the asymptotic expansion of the persistence threshold.*

The solution to Problem 4.1 is given in Appendix C.

Next, we show the existence of a unique root μ_0 to (4.53) on a certain interval with $\mu_0 > 0$ to be determined. Since $\int_\Omega m\, dx < 0$ from (4.50), it follows that $\mathcal{B}(0) < 0$ from (4.53). In addition, $\mathcal{B}(\mu_0) \to +\infty$ as $\mu_0 \to 2/(m_J \rho_J^2)$ from below, where $m_J \rho_J^2$ is defined by

$$m_J \rho_J^2 = \max_{m_j > 0} \{ m_j \rho_j^2 \,|\, j = 1, \ldots, n \} . \tag{4.57}$$

There must be at least one j for which $m_j > 0$, so that (4.57) is attained at some $j = J$. Moreover, (4.53) readily yields that $\mathcal{B}'(\mu_0) > 0$ on $0 < \mu_0 < 2/(m_J \rho_J^2)$. Therefore, there exists a unique root $\mu_0 = \mu_0^\star$ on $0 < \mu_0 < 2/(m_J \rho_J^2)$ to $\mathcal{B}(\mu_0) = 0$. The corresponding leading-order eigenfunction in the inner region, ψ_{0j}, satisfies $\psi_{0j} > 0$ from (C.10). Therefore, $\mu_0^\star$ is the leading-order term in the asymptotic expansion of the positive principal eigenvalue of (4.49).

In this section, the formulae derived in §2 and §3 for the persistence threshold, $\lambda(\varepsilon)$, are used to determine the optimal strategy for distributing a fixed quantity of resources in some domain where favorable and unfavorable patches may already be present. The constraint that the resources being distributed are fixed is expressed mathematically by

$$-m_b |\Omega| + \frac{\pi}{2} \sum_{j=1}^{n} \alpha_j m_j \rho_j^2 + \mathcal{O}(\varepsilon^2) = \int_\Omega m\, dx = -K \,, \tag{4.58}$$

where $K > 0$ is kept constant as m_b, or α_j, m_j, and ρ_j, for $j = 1, \ldots, n$ are varied.

We first consider the case of one favorable habitat. For an interior patch of area $\pi\varepsilon^2$, we recall that λ is given in (4.31 a) of Principal Result 4.1. For a boundary patch of the same area, we must set $\pi \alpha_0 \varepsilon^2 \rho_0^2 / 2 = \pi \varepsilon^2$ in (4.48 a) of Principal Result 4.2. Thus, $\rho_0 = \sqrt{2/\alpha_0}$, so that (4.48 a) becomes

$$\lambda = \mu_0 \nu - \mu_0 \nu^2 \left[\frac{1}{4} + \alpha_0 \pi R_s(x_0; x_0) - \frac{1}{2} \log \left(\frac{2}{\alpha_0} \right) \right] + \mathcal{O}(\nu^3) \,; \qquad \mu_0 \equiv \frac{\alpha_0}{m_+} \left[1 - \frac{\pi m_+}{|\Omega| m_b} \right] . \tag{4.59}$$

By comparing the leading-order $\mathcal{O}(\nu)$ terms in (4.59) and (4.31 a), and noting that $\alpha_0 < 2$ for a boundary patch, we obtain the following main result:

Qualitative Result I: *For a favorable habitat of area $\pi\varepsilon^2$, the positive principal eigenvalue λ is always smaller for a boundary patch than for an interior patch. For a domain boundary with corners, λ is minimized when the boundary patch is centered at the corner with the smallest corner contact angle $\pi\alpha_0$, as opposed to a patch on the smooth part of the boundary, only if $\alpha_0 < 1$. For a domain with smooth boundary, for which $\alpha_0 = 1$ for any $x_0 \in \partial\Omega$, then λ in (4.59) is minimized when the center x_0 of the boundary patch is located at the global maximum of the regular part $R_s(x_0; x_0)$ of the surface Neumann Green's function of (4.44) on $\partial\Omega$. Thus, the movement of either a single favorable habitat to the boundary of the domain is advantageous for the persistence of the species*

Next, for a fixed value of the constraint in (4.58), we consider the effect of both the location and the fragmentation of resources on the leading-order term, μ_0, in the asymptotic expansion of λ in (4.52) of Principal Result 4.3. The analysis below leads to three specific qualitative results. The following simple lemma is central to the derivation of these results:

Lemma: *Consider two smooth functions $C_{old}(\zeta)$ and $C_{new}(\zeta)$ defined on $0 \leq \zeta < \mu_m^{old}$ and $0 \leq \zeta < \mu_m^{new}$, respectively, with $C_{old}(0) = C_{new}(0) < 0$, and $C_{old}(\zeta) \to +\infty$ as $\zeta \to \mu_m^{old}$ from below, and $C_{new}(\zeta) \to +\infty$ as $\zeta \to \mu_m^{new}$ from below. Suppose further that there exist unique roots $\zeta = \mu_0^{old}$ and $\zeta = \mu_0^{new}$ to $C_{old}(\zeta) = 0$ and $C_{new}(\zeta) = 0$ on the intervals $0 < \zeta < \mu_m^{old}$ and $0 < \zeta < \mu_m^{new}$, respectively. Then,*

- *Case I: If $\mu_m^{new} \leq \mu_m^{old}$ and $C_{new}(\zeta) > C_{old}(\zeta)$ on $0 < \zeta < \mu_m^{new}$, then $\mu_0^{new} < \mu_0^{old}$.*
- *Case II: If $\mu_m^{new} \geq \mu_m^{old}$ and $C_{new}(\zeta) < C_{old}(\zeta)$ on $0 < \zeta < \mu_m^{old}$, then $\mu_0^{new} > \mu_0^{old}$.*

The proof of this lemma is a routine exercise in calculus and is omitted. We now use this simple lemma to obtain our three main qualitative results.

First, we suppose that the center of the j^{th} patch of radius $\varepsilon\rho_j$ with associated angle $\pi\alpha_j$ is moved to an unoccupied location, with the new patch having radius $\varepsilon\rho_k$ and associated angle $\pi\alpha_k$. To satisfy (4.58), we require that $\alpha_j m_j \rho_j^2 = \alpha_k m_k \rho_k^2$. The change in $\mathcal{B}(\zeta)$, with $\mathcal{B}(\zeta)$ as defined in (4.53), induced by this action is

$$\mathcal{B}_{\text{new}}(\zeta) - \mathcal{B}_{\text{old}}(\zeta) = \frac{\pi\alpha_k m_k \rho_k^2}{2 - \zeta m_k \rho_k^2} - \frac{\pi\alpha_j m_j \rho_j^2}{2 - \zeta m_j \rho_j^2} = \pi \left(\frac{\alpha_j}{\alpha_k}\right) \frac{m_j^2 \rho_j^4 \zeta}{\left(2 - \zeta m_j \rho_j^2\right)\left(2 - \zeta m_k \rho_k^2\right)} (\alpha_j - \alpha_k) \,. \tag{4.60}$$

Recall from §3 that $\mathcal{B}_{\text{old}}(\zeta) = 0$ has a positive root $\zeta = \mu_0^{\text{old}}$ on $0 < \zeta < \mu_{\text{m}}^{\text{old}} \equiv 2/(m_J \rho_J^2)$, where $m_J \rho_J^2$ was defined in (4.57).

Assume that $\alpha_j > \alpha_k$. For instance, this occurs when the center of an interior patch, for which $\alpha_j = 2$, is moved to a smooth point on the domain boundary, for which $\alpha_k = 1$. First, suppose that the patches are favorable so that $m_j > 0$ and $m_k > 0$. When $\alpha_j > \alpha_k$, it follows from the constraint $\alpha_j m_j \rho_j^2 = \alpha_k m_k \rho_k^2$ that $m_k \rho_k^2 > m_j \rho_j^2$, and so the first vertical asymptote for $\mathcal{B}_{\text{new}}(\zeta)$ cannot be larger than that of $\mathcal{B}_{\text{old}}(\zeta)$. Consequently, we define $m_K \rho_K^2 \equiv \max\{m_J \rho_J^2, m_k \rho_k^2\}$, and from §3 we conclude that there is a unique root $\zeta = \mu_0^{\text{new}}$ to $\mathcal{B}_{\text{new}}(\zeta) = 0$ on $0 < \zeta < \mu_{\text{m}}^{\text{new}} \equiv 2/(m_K \rho_K^2)$. Since $\mu_{\text{m}}^{\text{new}} \leq \mu_{\text{m}}^{\text{old}}$, and (4.60) shows that $\mathcal{B}_{\text{new}}(\zeta) > \mathcal{B}_{\text{old}}(\zeta)$ for $0 < \zeta < \mu_{\text{m}}^{\text{new}}$, then Case I of the Lemma proves that $\mu_0^{\text{new}} < \mu_0^{\text{old}}$. Alternatively, for the situation where habitats are unfavorable, so that $m_j < 0$ and $m_k < 0$, then the first vertical asymptotes of $\mathcal{B}_{\text{old}}(\zeta)$ and $\mathcal{B}_{\text{new}}(\zeta)$ must be the same, since these asymptotes are defined only in terms of the favorable patches. For this case, (4.60) again shows that $\mathcal{B}_{\text{new}}(\zeta) > \mathcal{B}_{\text{old}}(\zeta)$ for $0 < \zeta < 2/(m_J \rho_J^2)$. Case I of Lemma then establishes that $\mu_0^{\text{new}} < \mu_0^{\text{old}}$. ■

Next, we consider the effect of fragmentation on species persistence. More specifically, we consider the effect of splitting the i^{th} patch, of radius $\varepsilon\rho_i$ and growth rate m_i, into two distinct patches, one with radius $\varepsilon\rho_j$ and growth rate m_j, and the other with radius $\varepsilon\rho_k$ and growth rate m_k. The condition $m_i \rho_i^2 = m_j \rho_j^2 + m_k \rho_k^2$ is imposed to satisfy the constraint (4.58). We assume that $\alpha_i = \alpha_j = \alpha_k$, so that we are either splitting an interior patch into two interior patches, or a boundary patch into two boundary patches, with each boundary patch centered at either a smooth point of $\partial\Omega$ or at a corner point of $\partial\Omega$ with the same contact angle. This action leads to the following qualitative result:

Qualitative Result II: *The fragmentation of one favorable interior habitat into two separate favorable interior habitats is not advantageous for species persistence. Similarly, the fragmentation of a favorable boundary habitat into two favorable boundary habitats with each either centered at either a smooth point of $\partial\Omega$, or at a corner point of $\partial\Omega$ with the same contact angle, is not advantageous. Finally, the fragmentation of an unfavorable habitat into two separate unfavorable habitats increases the persistence threshold λ.*

We prove this result for $\alpha_i = \alpha_j = \alpha_k$ as follows. First, consider the case where we are fragmenting one favorable habitat into two smaller favorable habitats. Then, $m_i > 0$, $m_j > 0$, and $m_k > 0$. For the original patch distribution, it follows from §3 that $\mathcal{B}_{\text{old}}(\zeta) = 0$ has a positive root $\zeta = \mu_0^{\text{old}}$ on $0 < \zeta < \mu_{\text{m}}^{\text{old}} \equiv 2/(m_J\rho_J^2)$, where $m_J\rho_J^2$ was defined in (4.57). Since, clearly, the first vertical asymptote for $\mathcal{B}_{\text{new}}(\zeta)$ cannot be smaller than that of $\mathcal{B}_{\text{old}}(\zeta)$ under this fragmentation, it follows from §3 that $\mathcal{B}_{\text{new}}(\zeta) = 0$ has a positive root $\zeta = \mu_0^{\text{new}}$ on $0 < \zeta < \mu_{\text{m}}^{\text{new}}$ with $\mu_{\text{m}}^{\text{new}} \geq \mu_{\text{m}}^{\text{old}}$. From (4.53), we then calculate under the constraint $m_i\rho_i^2 = m_j\rho_j^2 + m_k\rho_k^2$ that the change in $\mathcal{B}(\zeta)$ induced by this fragmentation action is

$$\mathcal{B}_{\text{new}}(\zeta) - \mathcal{B}_{\text{old}}(\zeta) = \frac{\pi\alpha_i m_j\rho_j^2}{(2-\zeta m_j\rho_j^2)} + \frac{\pi\alpha_i m_k\rho_k^2}{(2-\zeta m_k\rho_k^2)} - \frac{\pi\alpha_i m_i\rho_i^2}{(2-\zeta m_i\rho_i^2)}$$
$$= \frac{-\pi\alpha_i\zeta\left(m_j\rho_j^2 m_k\rho_k^2\right)\left[\left(2-\zeta m_j\rho_j^2\right) + \left(2-\zeta m_k\rho_k^2\right)\right]}{\left(2-\zeta m_i\rho_i^2\right)\left(2-\zeta m_j\rho_j^2\right)\left(2-\zeta m_k\rho_k^2\right)}. \tag{4.61}$$

Hence, from (4.61), we have that $\mathcal{B}_{\text{new}}(\zeta) < \mathcal{B}_{\text{old}}(\zeta)$ on $0 < \zeta < \mu_{\text{m}}^{\text{old}} \equiv 2/(m_J\rho_J^2)$. Since, in addition $\mu_{\text{m}}^{\text{new}} \geq \mu_{\text{m}}^{\text{old}}$, it follows from Case II of the Lemma that $\mu_0^{\text{new}} > \mu_0^{\text{old}}$. This proves the first two statements of Qualitative Result II.

To prove the final statement of this result, we suppose that we are fragmenting an unfavorable habitat into two smaller unfavorable habitats, so that $m_i < 0$, $m_j < 0$, and $m_k < 0$. For this situation, the first vertical asymptotes of $\mathcal{B}_{\text{old}}(\zeta)$ and $\mathcal{B}_{\text{new}}(\zeta)$ are the same, and (4.61) again shows that $\mathcal{B}_{\text{new}}(\zeta) < \mathcal{B}_{\text{old}}(\zeta)$ on $0 < \zeta < \mu_{\text{m}}^{\text{old}} \equiv 2/m_J\rho_J^2$. By Case II of the Lemma, we conclude that $\mu_0^{\text{new}} > \mu_0^{\text{old}}$, which proves the last statement of Qualitative Result II. ■

The combination of Qualitative Results I and II show that, given some fixed amount of favorable resources to distribute, the optimal strategy is to clump them all together at a point on the boundary of the domain, and more specifically at the corner point of the boundary (if any are present) with the smallest contact angle less than π degrees. This strategy will ensure that the value of μ_0, and consequently the leading-order term for λ, is as small as possible, thereby maximizing the range of diffusivities D in (4.1) for the persistence of the species.

Our final qualitative result addresses whether it is advantageous to fragment a single interior favorable habitat into a smaller interior favorable habit together with a favorable boundary habitat. To study this situation, we introduce the constraint

$$m_i\rho_i^2 = m_j\rho_j^2 + \frac{\alpha_k}{2}m_k\rho_k^2\,, \tag{4.62}$$

with $\alpha_i = \alpha_j = 2$, and $\alpha_k < 2$. The subscript i represents the original interior habitat, whereas j and k represent the new smaller interior habitat and new boundary habitat, respectively. It is not clear apriori whether this action is advantageous, given that fragmentation of a favorable interior habitat into two favorable interior habitats increases the persistence threshold λ, but the relocation of a favorable interior habitat to the boundary decreases λ. A sufficient condition to treat this case, together with two additional related results, are summarized as follows:

Qualitative Result III: *The fragmentation of one favorable interior habitat into a new smaller interior favorable habitat together with a favorable boundary habitat, is advantageous for species persistence when the boundary habitat is sufficiently strong in the sense that*

$$m_k \rho_k^2 > \frac{4}{2-\alpha_k} m_j \rho_j^2 > 0 \,. \tag{4.63}$$

Such a fragmentation of a favorable interior habitat is not advantageous when the new boundary habitat is too weak in the sense that

$$0 < m_k \rho_k^2 < m_j \rho_j^2 \,. \tag{4.64}$$

Finally, the clumping of a favorable boundary habitat and an unfavorable interior habitat into one single interior habitat is not advantageous for species persistence when the resulting interior habitat is still unfavorable.

Problem 4.3: *Give the proof of Qualitative Result III* (the solution is given in Appendix C).

Further results for the optimization of the persistence threshold in patchy environments are discussed in [**45**].

There are two key problems that warrant further study. Firstly, it is highly desirable to provide a rigorous derivation of the asymptotic expansion for λ in Principal Result 4.3. Such a derivation could possibly be based on variational considerations and gamma convergence theory, similar to that used in [**13**] (see also the references therein) to analyze bubble solutions for the Cahn-Hillard equation of phase transition theory. Secondly, it would be interesting to extend our single-species analysis to the case of multi-species interaction, such as predator-prey interactions, for which a partial fragmentation of the prey habitat may become more beneficial for the persistence of the prey, rather than clumping the prey into a single habitat.

4.2 The Narrow Escape Problem From a Sphere

The narrow escape problem concerns the motion of a Brownian particle confined in a bounded domain $\Omega \in R^d$ ($d = 2, 3$) whose boundary $\partial\Omega = \partial\Omega_r \cup \partial\Omega_a$ is almost entirely reflecting ($\partial\Omega_r$), except for small absorbing windows, or traps, labeled collectively by $\partial\Omega_a$, through which the particle can escape. Denoting the trajectory of the Brownian particle by $X(t)$, the mean first passage time (MFPT) $v(x)$ is defined as the expectation value of the time τ taken for the Brownian particle to become absorbed somewhere in $\partial\Omega_a$ starting initially from $X(0) = x \in \Omega$, so that $v(x) = E[\tau \,|\, X(0) = x]$. The calculation of $v(x)$ becomes a narrow escape problem in the limit when the measure of the absorbing set $|\partial\Omega_a| = \mathcal{O}(\varepsilon^{d-1})$ is asymptotically small, where $0 < \varepsilon \ll 1$ measures the dimensionless radius of an absorbing window. Since the MFPT diverges as $\varepsilon \to 0$, the calculation of the MFPT $v(x)$ constitutes a singular perturbation problem.

In a three-dimensional bounded domain Ω, it is well-known (cf. [**57**]) that the MFPT $v(x)$ satisfies a Poisson equation with mixed Dirichlet-Neumann boundary conditions, formulated as

$$\triangle v = -\frac{1}{D}\,, \qquad x \in \Omega\,, \tag{4.65 a}$$

$$v = 0\,, \qquad x \in \partial\Omega_a = \cup_{j=1}^{N} \partial\Omega_{\varepsilon_j}\,, \quad j = 1, \ldots, N\,; \qquad \partial_n v = 0\,, \qquad x \in \partial\Omega_r\,. \tag{4.65 b}$$

Here D is the diffusivity of the underlying Brownian motion, and the absorbing set consists of N small disjoint absorbing windows, or traps, $\partial\Omega_{\varepsilon_j}$ for $j = 1, \ldots, N$ each of area $|\partial\Omega_{\varepsilon_j}| = \mathcal{O}(\varepsilon^2)$. We assume that $\partial\Omega_{\varepsilon_j} \to x_j$ as $\varepsilon \to 0$ for $j = 1, \ldots, N$, and that the traps are well-separated in the sense that $|x_i - x_j| = \mathcal{O}(1)$ for all $i \neq j$. With respect to a uniform distribution of initial points $x \in \Omega$ for the Brownian walk, the average MFPT, denoted by $\bar{v}$, is defined by

$$\bar{v} = \chi \equiv \frac{1}{|\Omega|} \int_{\Omega} v(x)\, dx\,, \tag{4.66}$$

where $|\Omega|$ is the volume of Ω. The geometry of a confining sphere with traps on its boundary is depicted in Fig. 7.

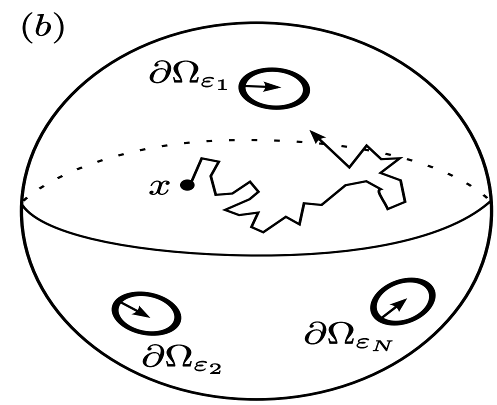


FIGURE 7. Sketch of a Brownian trajectory in the unit sphere in $\mathbb{R}^3$ with absorbing windows on the boundary.

There are only a few results for the MFPT, defined by (4.65), for a bounded three-dimensional domain. For the case of one locally circular absorbing window of radius ε on the boundary of the unit sphere, it was shown in [**65**] (with a correction as noted in [**67**]) that a two-term expansion for the average MFPT is given by

$$\bar{v} \sim \frac{|\Omega|}{4\varepsilon D} \left[1 - \frac{\varepsilon}{\pi} \log \varepsilon + \mathcal{O}(\varepsilon) \right]\,, \tag{4.67}$$

where $|\Omega|$ denotes the volume of the unit sphere. This result was derived in [**65**] by using Collins' method for solving a certain pair of integral equations resulting from a separation of variables approach. A similar result for $\bar{v}$ was obtained in [**65**] for the case of one small elliptical-shaped absorbing window on the boundary of a sphere. For an arbitrary three-dimensional bounded domain with one locally circular absorbing window of radius ε on its smooth boundary, it was shown in [**67**] that

$$\bar{v} \sim \frac{|\Omega|}{4\varepsilon D} \left[1 - \frac{\varepsilon}{\pi} H \log \varepsilon + \mathcal{O}(\varepsilon) \right]\,, \tag{4.68}$$

where H denotes the mean curvature of the domain boundary at the center of the absorbing window. In [**30**] an approximate analytical theory was developed to determine the average MFPT for the case of two circular absorbing windows on the boundary of the unit sphere, with arbitrary window separation. For this two-window case, the average

MFPT was determined in terms of an integral and an unspecifed $\mathcal{O}(1)$ term, which was estimated from Brownian particle simulations.

In [**15**] this previous work was extended to calculate a a three-term asymptotic expansion for the MFPT for the case of N small locally circular absorbing windows, or traps, on the boundary of the unit sphere. This three-term asymptotic expansion for the MFPT shows explicitly the significant effects of both the fragmentation of the trap set and the spatial arrangement of the traps on the boundary of the sphere. For the special case where the N traps have a common radius $\varepsilon \ll 1$, and are centered at x_j with $|x_j| = 1$ for $j = 1, \ldots, N$ and $|x_i - x_j| = \mathcal{O}(1)$ for $i \neq j$, the results in [**15**] show that the average MFPT has the three-term asymptotic expansion

$$\bar{v} = \frac{|\Omega|}{4\varepsilon DN}\left[1 + \frac{\varepsilon}{\pi}\log\left(\frac{2}{\varepsilon}\right) + \frac{\varepsilon}{\pi}\left(-\frac{9N}{5} + 2(N-2)\log 2 + \frac{3}{2} + \frac{4}{N}\mathcal{H}(x_1, \ldots, x_N)\right) + \mathcal{O}(\varepsilon^2 \log \varepsilon)\right], \tag{4.69 a}$$

where the discrete energy-like function $\mathcal{H}(x_1, \ldots, x_N)$ is defined by

$$\mathcal{H}(x_1, \ldots, x_N) = \sum_{\substack{j=1 \\ j \neq i}}^{K}\left(\frac{1}{|x_i - x_j|} - \frac{1}{2}\log|x_i - x_j| - \frac{1}{2}\log\left(2 + |x_i - x_j|\right)\right). \tag{4.69 b}$$

The asymptotic analysis in [**15**] leading to (4.69) relies on two essential ingredients. Firstly, it requires detailed properties of the surface Neumann Green's function for the unit sphere and, in particular, the determination of both the subdominant logarithmic singularity and the regular part of this function. The identification of a weak logarithmic singularity for this Green's function was first made in [**34**] for the unit sphere, and for a general three-dimensional domain in [**54**], [**61**], and [**67**]. Secondly, the analysis in [**15**] requires the introduction of certain logarithmic switchback terms that commonly occur in the asymptotic analysis of certain problems in fluid mechanics (see [**42**] for a discussion of logarithmic switchback terms). Further we remark that the analysis is rather complicated owing to the fact that one must determine the far-field behavior of a rather difficult inhomogeneous problem that arises at a higher order in the asymptotic expansion.

We now highlight the steps in the asymptotic analysis of [**15**] leading to (4.69). We assume that there are N small well-separated windows on the boundary of the sphere centered at x_j with $j = 1, \ldots, N$ where $|x_j| = 1$. Each window is assumed to have a circular projection onto the tangent plane to the sphere at x_j and has a radius of εa_j where $\varepsilon \ll 1$. The problem for the MFPT $v = v(x)$, written in spherical coordinates, is

$$\triangle v \equiv v_{rr} + \frac{2}{r}v_r + \frac{1}{r^2\sin^2\theta}v_{\phi\phi} + \frac{\cot\theta}{r^2}v_\theta + \frac{1}{r^2}v_{\theta\theta} = -\frac{1}{D}, \qquad r = |x| \leq 1, \tag{4.70 a}$$

$$v = 0, \qquad x \in \partial\Omega_a = \cup_{j=1}^{N}\partial\Omega_{\varepsilon_j}, \quad j = 1, \ldots, N; \qquad \partial_r v = 0, \qquad x \in \partial\Omega \backslash \partial\Omega_a. \tag{4.70 b}$$

Here each $\partial\Omega_{\varepsilon_j}$ for $j = 1, \ldots, N$ is a small "circular" cap centered at (θ_j, ϕ_j) defined by

$$\partial\Omega_{\varepsilon_j} \equiv \{(\theta, \phi) \mid (\theta - \theta_j)^2 + \sin^2(\theta_j)(\phi - \phi_j)^2 \leq \varepsilon^2 a_j^2\}. \tag{4.70 c}$$

The area of $\partial\Omega_{\varepsilon_j}$ is $|\partial\Omega_{\varepsilon_j}| \sim \pi\varepsilon^2 a_j^2$. In (4.70 a), $0 \leq \phi \leq 2\pi$ is the longitude, $0 \leq \theta \leq \pi$ is the latitude, and the center of the j^{th} window is at $x_j \in \partial\Omega$ where $|x_j| = 1$ for $j = 1, \ldots, N$.

To solve (4.70) asymptotically, we first must calculate the surface Neumann Green's function. For the unit sphere

Ω with volume $|\Omega| = 4\pi/3$, the surface Neumann Green's function $G_s(x; x_j)$ satisfies

$$\triangle G_s = \frac{1}{|\Omega|}\,, \quad x \in \Omega\,; \qquad \partial_r G_s = \delta(\cos\theta - \cos\theta_j)\delta(\phi - \phi_j)\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega G_s\, dx = 0\,. \tag{4.71}$$

In terms of spherical coordinates, the points $x \in \partial\Omega$, $x_j \in \partial\Omega$, and the dot product $x \cdot x_j$, are given by

$$x = (\cos\phi \sin\theta,\, \sin\phi \sin\theta,\, \cos\theta)\;, \qquad x_j = (\cos\phi_j \sin\theta_j,\, \sin\phi_j \sin\theta_j,\, \cos\theta_j)\;, \qquad \cos\gamma = x \cdot x_j\,, \tag{4.72}$$

where γ denotes the angle between x and x_j given by $\cos\gamma = \cos\theta\cos\theta_j + \sin\theta\sin\theta_j\cos(\phi - \phi_j)$. The following result for $G_s(x; x_j)$ is derived in Appendix A of [**15**].

Lemma: *For the unit sphere, the surface Neumann Green's function satisfying (4.71) is given explicitly by*

$$G_s(x; x_j) = \frac{1}{2\pi\,|x - x_j|} + \frac{1}{8\pi}\left(|x|^2 + 1\right) + \frac{1}{4\pi}\log\left(\frac{2}{1 - |x|\cos\gamma + |x - x_j|}\right) - \frac{7}{10\pi}\,. \tag{4.73}$$

The calculations below for the MFPT require the limiting behavior of G_s in (4.73) as $x \to x_j \in \partial\Omega$ when expressed in terms of a local coordinate system (η, s_1, s_2) whose origin is at the center of the j^{th} absorbing window. We define the local cartesian coordinate, y, together with the local curvilinear coordinates η, s_1, and s_2 by

$$y \equiv \varepsilon^{-1}(x - x_j)\,, \qquad \eta \equiv \varepsilon^{-1}(1 - r)\,, \qquad s_1 \equiv \varepsilon^{-1}\sin(\theta_j)\,(\phi - \phi_j)\;, \qquad s_2 \equiv \varepsilon^{-1}(\theta - \theta_j)\,. \tag{4.74}$$

From the law of cosines we calculate that

$$1 - |x|\cos\gamma = \frac{1}{2}\left[|x - x_j|^2 - \left(|x|^2 - 1\right)\right] \sim \frac{1}{2}\left[\mathcal{O}(\varepsilon^2) - \left((1 - \varepsilon\eta)^2 - 1\right)\right] \sim \varepsilon\eta + \mathcal{O}(\varepsilon^2)\,. \tag{4.75}$$

Therefore, upon substituting (4.75) and (4.74) into (4.73), we obtain as $x \to x_j$ that

$$G_s(x; x_j) = \frac{1}{2\pi\varepsilon\,|y|} - \frac{1}{4\pi}\log\left(\frac{\varepsilon}{2}\right) - \frac{1}{4\pi}\log\left(|y| + \eta\right) - \frac{9}{20\pi} + \mathcal{O}(\varepsilon)\,. \tag{4.76}$$

The weak logarithmic singularity in (4.76) on $\eta = 0$ was observed previously for the sphere in [**34**] (see page 247 of [**34**]), and for general domains in [**61**], [**54**], and [**67**]. The calculation in Appendix A of [**15**] identifies the regular part of the singularity structure for G_s in (4.76), which is needed below to obtain a three-term expansion for the MFPT.

By retaining linear and quadratic terms for the mapping $x - x_j \mapsto (\eta, s_1, s_2)$, a lengthy but straightforward calculation, which we omit, shows that for $x \to x_j$

$$\frac{1}{|y|} = \frac{1}{\rho} + \frac{\varepsilon}{2\rho^3}\left[\eta(s_1^2 + s_2^2) - s_1^2 s_2 \cot\theta_j\right] + \mathcal{O}(\varepsilon^2)\,, \qquad \rho \equiv \left(\eta^2 + s_1^2 + s_2^2\right)^{1/2}\,. \tag{4.77}$$

In order to obtain the local representation of the surface Neumann Green's function with an error of $\mathcal{O}(\varepsilon)$, as required for the asymptotic analysis below, we substitute (4.77) into (4.76) to obtain for $x \to x_j$ that

$$G_s(x; x_j) = \frac{1}{2\pi\varepsilon\rho} - \frac{1}{4\pi}\log\left(\frac{\varepsilon}{2}\right) + \frac{1}{4\pi}\left[\frac{\eta(s_1^2 + s_2^2)}{\rho^3} - \frac{s_1^2 s_2 \cot\theta_j}{\rho^3}\right] - \frac{1}{4\pi}\log\left(\rho + \eta\right) - \frac{9}{20\pi} + \mathcal{O}(\varepsilon)\,. \tag{4.78}$$

We now solve (4.70) in the limit $\varepsilon \to 0$ by using the method of matched asymptotic expansions. In the outer region away from the absorbing windows we expand the outer solution as

$$v \sim \varepsilon^{-1}v_0 + v_1 + \varepsilon\log\left(\frac{\varepsilon}{2}\right)v_2 + \varepsilon v_3 + \cdots\,. \tag{4.79}$$

Here v_0 is an unknown constant, while v_1, v_2, and v_3 are functions to be determined. As shown below, the third non-analytic term in ε in (4.79) arises as a result of the term in (4.78) with logarithmic dependence on ε. In addition, we show below that one must add a further term of the form $\log(\varepsilon/2)\,\chi_0$ directly between the first and second terms in (4.79), where χ_0 is a certain constant. Such terms are called switchback terms in singular perturbation theory, and they have a long history in the study of certain ODE and PDE models in fluid mechanics (cf. [**42**]).

We first substitute (4.79) into (4.70) to obtain that v_k, for $k = 1, \ldots, 3$, satisfies

$$\triangle v_k = -\frac{1}{D}\delta_{k1}\,, \qquad x \in \Omega\,; \qquad \partial_n v_k = 0\,, \qquad x \in \partial\Omega\backslash\{x_1, \ldots, x_N\}\,, \tag{4.80}$$

where $\delta_{k1} = 1$ if $k = 1$ and $\delta_{k1} = 0$ for $k > 1$. The analysis below yields appropriate singularity behaviors for each v_k as $x \to x_j$, for $j = 1, \ldots, N$. In the inner region near the j^{th} absorbing window we introduce the local coordinates (η, s_1, s_2) as defined in (4.74), and we pose the inner expansion

$$v \sim \varepsilon^{-1} w_0 + \log\left(\frac{\varepsilon}{2}\right) w_1 + w_2 + \cdots\,. \tag{4.81}$$

We substitute (4.81) into (4.70) after first transforming (4.70 a) in terms of the local coordinate system (4.74) as outlined in Appendix B. In the limit $\varepsilon \to 0$, this yields a sequence of problems for w_k for $k = 0, 1, 2$ given by

$$\mathcal{L} w_k \equiv w_{k\eta\eta} + w_{k s_1 s_1} + w_{k s_2 s_2} = \delta_{k2}\ \mathcal{F}_2\,, \qquad \eta \geq 0\,, \quad -\infty < s_1, s_2 < \infty\,, \tag{4.82 a}$$

$$\partial_\eta w_k = 0\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \geq a_j^2\,; \qquad w_k = 0\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \leq a_j^2\,, \tag{4.82 b}$$

where $\delta_{22} = 1$ and $\delta_{k2} = 0$ if $k = 0, 1$. In (4.82 a) $\mathcal{F}_2$, is defined by

$$\mathcal{F}_2 \equiv 2\left(\eta w_{0\eta\eta} + w_{0\eta}\right) - \cot\theta_j\left(w_{0s_2} - 2s_2 w_{0s_1s_1}\right)\,, \qquad \eta \geq 0\,, \quad -\infty < s_1, s_2 < \infty\,. \tag{4.82 c}$$

The leading order matching condition is that $w_0 \sim v_0$ as $\rho \equiv (\eta^2 + s_1^2 + s_2^2)^{1/2} \to \infty$. Therefore, we write

$$w_0 = v_0\left(1 - w_c\right)\,, \tag{4.83}$$

where v_0 is a constant to be determined, and w_c is the solution satisfying $w_c \to 0$ as $\rho \to \infty$ to

$$\mathcal{L} w_c = 0\,, \qquad \eta \geq 0\,, \quad -\infty < s_1, s_2 < \infty\,, \tag{4.84 a}$$

$$\partial_\eta w_c = 0\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \geq a_j^2\,; \qquad w_c = 1\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \leq a_j^2\,. \tag{4.84 b}$$

This is the well-known electrified disk problem in electrostatics (cf. [**31**]), whose solution is (see page 38 of [**24**])

$$w_c = \frac{2}{\pi}\int_0^\infty \frac{\sin\mu}{\mu}\, e^{-\mu\eta/a_j}\, J_0\left(\frac{\mu\sigma}{a_j}\right) d\mu = \frac{2}{\pi}\sin^{-1}\left(\frac{a_j}{L}\right)\,, \qquad \sigma \equiv (s_1^2 + s_2^2)^{1/2}\,, \tag{4.85 a}$$

where $J_0(z)$ is the Bessel function of the first kind of order zero, and $L = L(\eta, \sigma)$ is defined by

$$L(\eta, \sigma) \equiv \frac{1}{2}\left(\left[(\sigma + a_j)^2 + \eta^2\right]^{1/2} + \left[(\sigma - a_j)^2 + \eta^2\right]^{1/2}\right)\,. \tag{4.85 b}$$

From either an asymptotic expansion of the integral representation of w_c using Laplace's method or, alternatively, from a direct calculation of the simple exact solution for w_c given in (4.85 a), we readily obtain the far-field behavior

$$w_c \sim \frac{2a_j}{\pi}\left(\frac{1}{\rho} + \frac{a_j^2}{6}\left(\frac{1}{\rho^3} - \frac{3\eta^2}{\rho^5}\right) + \cdots\right)\,, \quad \text{as} \quad \rho \to \infty\,, \tag{4.86}$$

which is uniformly valid in η, s_1, and s_2. Therefore, from (4.83) and (4.86), the far-field expansion for w_0 is

$$w_0 \sim v_0 \left(1 - \frac{c_j}{\rho} + \mathcal{O}(\rho^{-3}) \right) , \quad \text{as} \quad \rho \to \infty , \qquad c_j \equiv \frac{2a_j}{\pi} , \tag{4.87}$$

where c_j is the electrostatic capacitance of the circular disk of radius a_j. Next, we write the matching condition that the near-field behavior of the outer expansion (4.79) must agree with the far-field behavior of the inner expansion (4.81), so that

$$\frac{v_0}{\varepsilon} + v_1 + \varepsilon \log\left(\frac{\varepsilon}{2}\right) v_2 + \varepsilon v_3 + \cdots \sim \frac{v_0}{\varepsilon} \left(1 - \frac{c_j}{\rho} \cdots \right) + \log\left(\frac{\varepsilon}{2}\right) w_1 + w_2 + \cdots . \tag{4.88}$$

Therefore, since $\rho \sim \varepsilon^{-1}|x - x_j|$, we obtain that v_1 must satisfy (4.80) with the singular behavior $v_1 \sim -v_0 c_j / |x - x_j|$ as $x \to x_j$ for $j = 1, \ldots, N$. This problem for v_1 can be written in distributional form as

$$\triangle v_1 = -\frac{1}{D} , \qquad x \in \Omega ; \qquad \partial_r v_1|_{r=1} = -2\pi v_0 \sum_{j=1}^{N} \frac{c_j}{\sin\theta_j} \delta(\theta - \theta_j)\delta(\phi - \phi_j) . \tag{4.89}$$

By applying the divergence theorem, (4.89) has a solution only when v_0 is given by

$$v_0 = \frac{|\Omega|}{2\pi D N \bar{c}} , \qquad \bar{c} \equiv \frac{1}{N} \sum_{j=1}^{N} c_j , \qquad c_j = \frac{2a_j}{\pi} . \tag{4.90}$$

Thus, the solvability condition for the problem for v_1 determines the unknown leading-order constant term v_0 in the outer expansion. The solution to (4.89) is then written as a superposition over the surface Neumann Green's function $G_s(x; x_j)$, with $\int_\Omega G_s(x; x_j)\, dx = 0$, together with an unknown constant χ, as

$$v_1 = -2\pi v_0 \sum_{i=1}^{N} c_i G_s(x; x_i) + \chi , \qquad \chi \equiv |\Omega|^{-1} \int_\Omega v_1 \, dx . \tag{4.91}$$

Next, we expand v_1 as $x \to x_j$ by using the near-field expansion of the surface Neumann Green's function given in (4.78). Upon substituting the resulting expression into the matching condition (4.88) we obtain

$$\begin{aligned} \frac{v_0}{\varepsilon} \left(1 - \frac{c_j}{\rho} \right) + \frac{v_0 c_j}{2} \log\left(\frac{\varepsilon}{2}\right) + \chi + \frac{v_0 c_j}{2} \left[\log(\eta + \rho) - \frac{\eta(s_1^2 + s_2^2)}{\rho^3} + \frac{s_1^2 s_2 \cot\theta_j}{\rho^3} \right] + B_j \\ + \varepsilon \log\left(\frac{\varepsilon}{2}\right) v_2 + \varepsilon v_3 + \cdots \sim \frac{v_0}{\varepsilon} \left(1 - \frac{c_j}{\rho} + \mathcal{O}(\rho^{-3}) \right) + \log\left(\frac{\varepsilon}{2}\right) w_1 + w_2 + \cdots . \end{aligned} \tag{4.92}$$

Here the constant B_j is defined by

$$B_j = -2\pi v_0 \left(-\frac{9}{20\pi} c_j + \sum_{\substack{j=1 \\ j \neq i}}^{N} c_i G_{sji} \right) , \qquad G_{sji} \equiv G_s(x_j; x_i) . \tag{4.93}$$

We compare the $\mathcal{O}(\log\varepsilon)$ terms on both sides of (4.92), which suggests that $w_1 \sim v_0 c_j/2$ as $\rho \to \infty$. However, this leads to a problem for v_2 with no solution. In order to obtain a solvable equation for v_2, we must write χ in the form

$$\chi = \log\left(\frac{\varepsilon}{2}\right) \chi_0 + \chi_1 , \tag{4.94}$$

where χ_0 and χ_1 are constants, independent of ε, to be found. This choice for χ is equivalent to inserting a constant term of order $\mathcal{O}(\log\varepsilon)$ between v_0 and v_1 in the outer expansion (4.79). With this choice of χ in (4.92), the matching condition (4.92) enforces that $w_1 \sim \chi_0 + v_0 c_j/2$ as $\rho \to \infty$. The solution w_1 to (4.82) that satisfies this far-field behavior is

$$w_1 = \left(\frac{v_0 c_j}{2} + \chi_0\right)(1 - w_c)\,, \tag{4.95}$$

where w_c, given explicitly in (4.85), is the solution to (4.84). Therefore, using (4.86), we obtain the far-field behavior

$$w_1 \sim \left(\frac{v_0 c_j}{2} + \chi_0\right)\left(1 - \frac{c_j}{\rho} + \mathcal{O}(\rho^{-3})\right)\,. \tag{4.96}$$

Next, we substitute (4.96) into the matching condition (4.92) and use $\rho \sim \varepsilon^{-1}|x - x_0|$. This yields that the solution v_2 to (4.80) has the singular behavior $v_2 \sim -\left(\frac{v_0 c_j}{2} + \chi_0\right) c_j/|x - x_j|$ as $x \to x_j$. Therefore, v_2 satisfie

$$\triangle v_2 = 0\,, \qquad x \in \Omega\,; \qquad \partial_r v_2|_{r=1} = -2\pi \sum_{j=1}^{N} c_j \left(\frac{v_0 c_j}{2} + \chi_0\right) \frac{\delta(\theta - \theta_j)\delta(\phi - \phi_j)}{\sin\theta_j}\,. \tag{4.97}$$

By using the divergence theorem, we obtain that (4.97) is solvable only when χ_0 is given by

$$\chi_0 = -\frac{v_0}{2N\bar{c}} \sum_{j=1}^{N} c_j^2\,. \tag{4.98}$$

Then, the solution for v_2 can be written in terms of the surface Neumann Green's function as

$$v_2 = -2\pi \sum_{i=1}^{N} c_i \left(\frac{v_0 c_i}{2} + \chi_0\right) G_s(x; x_i) + \chi_2\,. \tag{4.99}$$

Next, we match the $\mathcal{O}(1)$ terms in (4.92) with χ as given in (4.94). We obtain that w_2 satisfies (4.82) with the far-field behavior

$$w_2 \sim B_j + \chi_1 + \frac{v_0 c_j}{2}\left[\log(\eta + \rho) - \frac{\eta(s_1^2 + s_2^2)}{\rho^3}\right] + \left(\frac{v_0 c_j}{2\rho^3}\right) s_1^2 s_2 \cot\theta_j\,, \qquad \text{as} \quad \rho \to \infty\,. \tag{4.100}$$

By superposition, we decompose the solution to this problem for w_2 in the form

$$w_2 = (B_j + \chi_1)(1 - w_c) + v_0 w_{2e} + v_0 w_{2o}\,, \tag{4.101}$$

where w_c is the solution to the electrified disk problem (4.84). Upon writing $w_0 = v_0(1 - w_c)$ to calculate $\mathcal{F}_2$ in (4.82 *c*), we set w_{2e} to be the solution to

$$w_{2e\eta\eta} + w_{2es_1s_1} + w_{2es_2s_2} = -2w_{c\eta} - 2\eta w_{c\eta\eta}\,, \qquad \eta \geq 0\,, \quad -\infty < s_1, s_2 < \infty\,, \tag{4.102 a}$$

$$\partial_\eta w_{2e} = 0\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \geq a_j^2\,; \qquad w_{2e} = 0\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \leq a_j^2\,, \tag{4.102 b}$$

$$w_{2e} \sim \frac{c_j}{2}\log(\eta + \rho) - \frac{c_j}{2\rho^3}\eta(s_1^2 + s_2^2)\,, \quad \text{as} \quad \rho \to \infty\,. \tag{4.102 c}$$

Moreover, w_{2o} is taken to be the solution of

$$w_{2o\eta\eta} + w_{2os_1s_1} + w_{2os_2s_2} = \cot\theta_j\left(w_{cs_2} - 2s_2 w_{cs_1s_1}\right)\,, \qquad \eta \geq 0\,, \quad -\infty < s_1, s_2 < \infty\,, \tag{4.103 a}$$

$$\partial_\eta w_{2o} = 0\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \geq a_j^2\,; \qquad w_{2o} = 0\,, \quad \text{on} \quad \eta = 0\,,\ s_1^2 + s_2^2 \leq a_j^2\,, \tag{4.103 b}$$

$$w_{2o} \sim \frac{c_j}{2\rho^3} s_1^2 s_2 \cot\theta_j\,, \quad \text{as} \quad \rho \to \infty\,. \tag{4.103 c}$$

In Appendix B of [**15**] it is shown that the inhomogeneous terms given by the right-hand sides of (4.102 *a*) and (4.103 *a*) lead explicitly to the leading-order far-field asymptotic behavior as written in (4.102 *c*) and (4.103 *c*).

The solution v_1 in (4.91) involves an as yet unknown constant χ_1 from (4.94). In the determination of χ_1 below from a solvability condition applied to the problem for v_3, we must have identified all of the monopole terms of the form b/ρ as $\rho \to \infty$ for some constant b arising from the far-field behavior of each term in the decomposition (4.101) of w_2. It is only these monopole terms that give non-vanishing contributions in the solvability condition determining χ_1. Clearly, the first term $(B_j + \chi_1)(1 - w_c)$ in (4.101) yields a monopole term from (4.86). However, upon solving the problem for w_{2e} exactly as in Lemma B.1 of Appendix B of [**15**], it was found that w_{2e} also yields a monopole term, and it has the far-field behavior

$$w_{2e} = \frac{c_j}{2}\log(\eta+\rho) - \frac{c_j}{2\rho^3}\eta(s_1^2+s_2^2) - \frac{c_j\kappa_j}{\rho} + \mathcal{O}(\rho^{-2}), \quad \text{as} \quad \rho \to \infty, \tag{4.104}$$

where κ_j is given explicitly by

$$\kappa_j = \frac{c_j}{2}\left[2\log 2 - \frac{3}{2} + \log a_j\right]. \tag{4.105}$$

Alternatively, the solution w_{2o} to (4.103) is odd in s_2 and, hence, does not generate a monopole term at infinity. An explicit analytical solution for w_{2o} is given in Lemma B.2 of Appendix B of [**15**].

In this way, we obtain that the solution w_2 to (4.82) with leading-order far-field behavior (4.100) generates further terms in the far-field behavior of the form

$$w_2 \sim (B_j+\chi_1)\left(1-\frac{c_j}{\rho}\right) + \frac{v_0 c_j}{2}\left[\log(\eta+\rho) - \frac{\eta}{\rho^3}(s_1^2+s_2^2) + \frac{s_1^2 s_2}{\rho^3}\cot\theta_j - \frac{2\kappa_j}{\rho} + \mathcal{O}(\rho^{-2})\right], \quad \text{as} \quad \rho\to\infty. \tag{4.106}$$

Finally, we substitute (4.106) into the matching condition (4.92). The two monopole terms in (4.106) determine the singular behavior for the solution v_3 of (4.80) as

$$v_3 \sim -\frac{c_j\left(B_j+\chi_1+v_0\kappa_j\right)}{|x-x_j|} \qquad \text{as} \quad x \to x_j. \tag{4.107}$$

In distributional form, this problem for v_3 is equivalent to

$$\triangle v_3 = 0, \qquad x\in\Omega; \qquad \partial_r v_3|_{r=1} = -2\pi\sum_{j=1}^{N} c_j\left(B_j+\chi_1+v_0\kappa_j\right)\frac{\delta(\theta-\theta_j)\delta(\phi-\phi_j)}{\sin\theta_j}. \tag{4.108}$$

The solvability condition for (4.108), obtained by using the divergence theorem, determines χ_1 as

$$\chi_1 = -\frac{1}{N\bar{c}}\sum_{j=1}^{N} c_j\left[B_j + v_0\kappa_j\right]. \tag{4.109}$$

Then, upon using (4.93) for B_j, we can write χ_1 as the sum of two terms, one of which involves a quadratic form in terms of the capacitance vector $\mathcal{C}^T \equiv (c_1,\ldots,c_N)$, as

$$\chi_1 = \frac{2\pi v_0}{N\bar{c}}p_c(x_1,\ldots,x_N) - \frac{v_0}{N\bar{c}}\sum_{j=1}^{N} c_j\kappa_j, \qquad p_c(x_1,\ldots,x_N) \equiv \mathcal{C}^T\mathcal{G}_s\mathcal{C}. \tag{4.110}$$

Here κ_j is given in (4.105) and $\mathcal{G}_s$ is the Green's function matrix defined in terms of $G_s(x_i;x_j)$ by

$$\mathcal{G}_s \equiv \begin{pmatrix} R & G_{s12} & \cdots & G_{s1N} \\ G_{s21} & R & \cdots & G_{s2N} \\ \vdots & \vdots & \ddots & \vdots \\ G_{sN1} & \cdots & G_{sN,N-1} & R \end{pmatrix}, \qquad R = -\frac{9}{20\pi}, \quad G_{sij} \equiv G_s(x_i;x_j). \tag{4.111}$$

Finally, we substitute (4.90) for v_0 together with (4.91) for v_1, with χ as determined by (4.94), (4.98), and (4.110), into the outer expansion (4.79). This leads to the following main result:

Principal Result 4.4: *For $\varepsilon \to 0$, the asymptotic solution to (4.70) is given in the outer region $|x - x_j| \gg \mathcal{O}(\varepsilon)$ for $j = 1, \ldots, N$ by*

$$v = \frac{|\Omega|}{2\pi\varepsilon D N \bar{c}} \left[1 + \varepsilon \log\left(\frac{2}{\varepsilon}\right) \frac{\sum_{j=1}^N c_j^2}{2N\bar{c}} - 2\pi\varepsilon \sum_{j=1}^N c_j G_s(x; x_j) + \frac{2\pi\varepsilon}{N\bar{c}} p_c(x_1, \ldots, x_N) - \frac{\varepsilon}{N\bar{c}} \sum_{j=1}^N c_j \kappa_j + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right] . \tag{4.112}$$

Here $c_j = 2a_j/\pi$ is the capacitance of the j^{th} circular absorbing window of radius εa_j, $\bar{c} \equiv N^{-1}(c_1 + \ldots + c_N)$, $|\Omega| = 4\pi/3$, κ_j is defined in (4.105), $G_s(x; x_j)$ is the surface Neumann Green's function given in (4.73), and $p_c(x_1, \ldots, x_N)$ is the quadratic form defined in (4.110). Since $\int_\Omega G_s \, dx = 0$, then $\bar{v} = |\Omega|^{-1} \int_\Omega v \, dx$ is given by

$$\bar{v} = \frac{|\Omega|}{2\pi\varepsilon D N \bar{c}} \left[1 + \varepsilon \log\left(\frac{2}{\varepsilon}\right) \frac{\sum_{j=1}^N c_j^2}{2N\bar{c}} + \frac{2\pi\varepsilon}{N\bar{c}} p_c(x_1, \ldots, x_N) - \frac{\varepsilon}{N\bar{c}} \sum_{j=1}^N c_j \kappa_j + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right] . \tag{4.113}$$

For the case of one circular window of radius εa, we set $N = 1$, $c_1 = 2a/\pi$, and $a_1 = a$, in (4.112), (4.105), and (4.113) to get

$$\bar{v} = \frac{|\Omega|}{4\varepsilon a D} \left[1 + \frac{\varepsilon a}{\pi} \log\left(\frac{2}{\varepsilon a}\right) + \frac{\varepsilon a}{\pi} \left(-\frac{9}{5} - 2\log 2 + \frac{3}{2} \right) + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right] , \qquad v(x) = \bar{v} - \frac{|\Omega|}{D} G_s(x; x_1) . \tag{4.114}$$

For an initial position at the origin, i.e. $x = (0, 0)$, then with $G_s(0; x_1) = -3/(40\pi)$ from (4.73), (4.114) becomes

$$v(0) = \frac{|\Omega|}{4\varepsilon a D} \left[1 + \frac{\varepsilon a}{\pi} \log\left(\frac{2}{\varepsilon a}\right) - \frac{2\varepsilon a \log 2}{\pi} + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right] . \tag{4.115}$$

For the case of one circular absorbing window of radius ε (i.e. $a = 1$), it was derived in [**65**] that

$$\bar{v} \sim \frac{|\Omega|}{4\varepsilon D} \left[1 + \frac{\varepsilon}{\pi} \log\left(\frac{1}{\varepsilon}\right) + \mathcal{O}(\varepsilon) \right] . \tag{4.116}$$

The original result in equation (3.52) of [**65**] omits the π term in (4.116) due to an omission of an extra factor of π on the left-hand side of the equation above (3.52) of [**65**]. This was corrected in [**67**]. Our result (4.114) agrees asymptotically with that of (4.116) and determines the $\mathcal{O}(\varepsilon)$ term to $\bar{v}$ explicitly. More importantly, our main result in Principal Result 4.4 generalizes that of [**65**] to the case of N circular absorbing windows of different radii on the unit sphere, and provides the $\mathcal{O}(\varepsilon)$ term that accounts for the specific locations of the traps on the unit sphere.

A further interesting special case of Principal Result 4.4 is when there are N circular absorbing windows of a common radius ε. Then, upon setting $c_j = 2/\pi$, together with $a_j = 1$ for $j = 1, \ldots, N$ in (4.105), (4.113) reduces to

$$\bar{v} = \frac{|\Omega|}{4\varepsilon D N} \left[1 + \frac{\varepsilon}{\pi} \log\left(\frac{2}{\varepsilon}\right) + \frac{\varepsilon}{\pi} \left(-\frac{9}{5} + \frac{8\pi}{N} \sum_{\substack{j=1 \\ j \neq i}}^{K} G_s(x_i; x_j) - 2\log 2 + \frac{3}{2} \right) + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right] . \tag{4.117}$$

From (4.73), we readily calculate the interaction term $G_s(x_i; x_j)$ in (4.117) as

$$G_s(x_i; x_j) = -\frac{9}{20\pi} + \frac{1}{2\pi} \left(\frac{1}{|x_i - x_j|} - \frac{1}{2} \log\left[\sin^2\left(\frac{\gamma_{ij}}{2}\right) + \sin\left(\frac{\gamma_{ij}}{2}\right) \right] \right) , \qquad \cos(\gamma_{ij}) = x_i \cdot x_j \, , \tag{4.118}$$

where γ_{ij} denotes the angle between x_i and x_j. Therefore, (4.117) becomes

$$\bar{v} = \frac{|\Omega|}{4\varepsilon D N} \left[1 + \frac{\varepsilon}{\pi} \log\left(\frac{2}{\varepsilon}\right) + \frac{\varepsilon}{\pi} \left(-\frac{9N}{5} - 2\log 2 + \frac{3}{2} + \frac{4}{N} \tilde{\mathcal{H}}(x_1, \ldots, x_N) \right) + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right] , \tag{4.119 a}$$

where the discrete sum $\tilde{\mathcal{H}}(x_1,\ldots,x_N)$ with $|x_j|=1$ and $\cos\gamma_{ij}=x_i\cdot x_j$ for $i,j=1,\ldots,N$ is defined by

$$\tilde{\mathcal{H}}(x_1,\ldots,x_N)=\sum_{\substack{k=1\\k\neq i}}^{N}\left(\frac{1}{|x_i-x_j|}-\frac{1}{2}\log\left[\sin^2\left(\frac{\gamma_{ij}}{2}\right)+\sin\left(\frac{\gamma_{ij}}{2}\right)\right]\right). \qquad (4.119\,b)$$

Equivalently, we can write $\bar{v}$ in the alternative form

$$\bar{v}=\frac{|\Omega|}{4\varepsilon DN}\left[1+\frac{\varepsilon}{\pi}\log\left(\frac{2}{\varepsilon}\right)+\frac{\varepsilon}{\pi}\left(-\frac{9N}{5}+2(N-2)\log 2+\frac{3}{2}+\frac{4}{N}\mathcal{H}(x_1,\ldots,x_N)\right)+\mathcal{O}(\varepsilon^2\log\varepsilon)\right], \qquad (4.120\,a)$$

where $\mathcal{H}(x_1,\ldots,x_N)$ is defined by

$$\mathcal{H}(x_1,\ldots,x_N)=\sum_{\substack{j=1\\j\neq i}}^{K}\left(\frac{1}{|x_i-x_j|}-\frac{1}{2}\log|x_i-x_j|-\frac{1}{2}\log\left(2+|x_i-x_j|\right)\right). \qquad (4.120\,b)$$

The first term in $\mathcal{H}$ is the usual Coulomb singularity in three-dimensions, whereas the second term in (4.120 b) represents a contribution from surface diffusion on the boundary of the sphere, similar to that studied in [**19**].

As a remark, for the case of N circular absorbing windows of a common radius ε, the average MFPT, $\bar{v}$, is minimized in the limit $\varepsilon\to 0$ at the trap configuration $\{x_1\ldots,x_N\}$ that minimizes the discrete sum $\mathcal{H}(x_,\ldots,x_N)$ on the unit sphere $|x_j|=1$ for $j=1,\ldots,N$. The classic discrete variational problems of minimizing either the Coulomb energy $\sum_{\substack{j=1\\j\neq i}}^{K}|x_i-x_j|^{-1}$ or the logarithmic energy $-\sum_{\substack{j=1\\j\neq i}}^{K}\log|x_i-x_j|$ on the unit sphere has a long history in approximation theory (see [**55**], [**56**], [**41**], [**27**], and the references therein)..

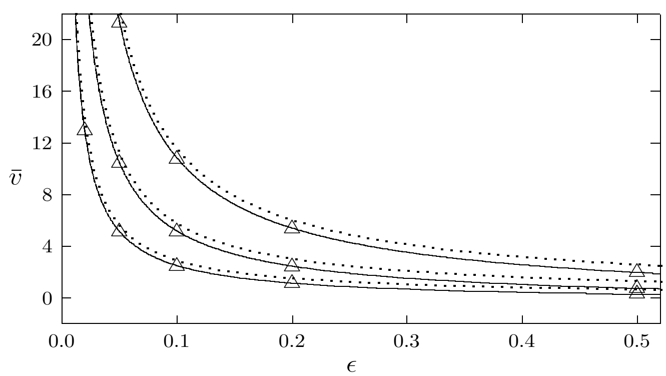


FIGURE 8. Plot of the average MFPT $\bar{v}$ versus ε from (4.120) with $D=1$ for either one, two, or four, identical windows on the surface of the unit sphere. The solid curves are the three-term expansion from (4.120) while the dotted curves are the truncation of (4.120) to two terms. The triangles denote the full numerical results computed from COMSOL [**17**]. Top curves: $N=1$. Middle curves: $N=2$ with antipodal windows. Bottom curves: $N=4$ with windows at the north and south poles, and two windows equally spaced on the equator.

Next, we validate our asymptotic result (4.120) with full numerical results. In Fig. 8 we compare our asymptotic results for the average MFPT $\bar{v}$ versus ε with those computed from full numerical simulations using the COMSOL finite element package [**17**]. The comparisons are done for $N=1$, $N=2$, and $N=4$, identical traps equally spaced on the surface of the unit sphere (see the caption of Fig. 8). Table 5 compares the two-term and three-term predictions for $\bar{v}$ from (4.120) with corresponding full numerical results computed using COMSOL. Note that the three-term expansion for $\bar{v}$ in (4.120) agrees well with full numerical results even when $\varepsilon=0.5$. For $\varepsilon=0.5$ and $N=4$, we

	$N = 1$			$N = 2$			$N = 4$		
ε	$\bar{v}_2$	$\bar{v}_3$	$\bar{v}_n$	$\bar{v}_2$	$\bar{v}_3$	$\bar{v}_n$	$\bar{v}_2$	$\bar{v}_3$	$\bar{v}_n$
0.02	53.89	53.33	52.81	26.95	26.42	26.12	13.47	13.11	12.99
0.05	22.17	21.61	21.35	11.09	10.56	10.43	5.54	5.18	5.12
0.10	11.47	10.91	10.78	5.74	5.21	5.14	2.87	2.51	2.47
0.20	6.00	5.44	5.36	3.00	2.47	2.44	1.50	1.14	1.13
0.50	2.56	1.99	1.96	1.28	0.75	0.70	0.64	0.28	0.30

Table 5. Comparison of asymptotic and full numerical results for $\bar{v}$ for either $N = 1$, $N = 2$, or $N = 4$, identical circular windows of radius ε equidistantly placed on the surface of the unit sphere (see the caption of Fig. 8). Here $\bar{v}_2$ is the two-term asymptotic result obtained by omitting the $\mathcal{O}(\varepsilon)$ term in (4.120), $\bar{v}_3$ is the three-term asymptotic result of (4.120), and $\bar{v}_n$ is the full numerical result computed from COMSOL [**17**].

calculate $N\pi\varepsilon^2/(4\pi) \approx 0.20$, so that the absorbing windows occupy roughly 25% of the surface area of the unit sphere. For this challenging test of perturbation theory, the last row and last three columns in Table 5 show that the three-term asymptotic result for the average MFPT differs from the full numerical result by only about 10%.

In [**15**], the main result in Principal Result 4.4 was used to study the effect of the fragmentation of the trap set. In addition, a scaling law for the minimum of the disrete energy for large N was derived by formally obtaining the form of this energy, and then fitting the coefficients in the expansion to numerical data computed from the numerical optimization code [**26**]. The result in [**15**] for $N \gg 1$ showed that the optimum $\mathcal{H}$ has the form

$$\mathcal{H} \approx \mathcal{F}(N) = \frac{N^2}{2}(1 - \log 2) + b_1 N^{3/2} + b_2 N \log N + b_3 N + b_4 N^{1/2} + b_5 \log N + b_6 \,, \tag{4.121 a}$$

The resulting least squares fit of (4.121 a) to numerical optimization data (see [**15**]) is

$$b_1 \approx -0.5668 \,, \quad b_2 \approx 0.0628 \,, \quad b_3 \approx -0.8420 \,, \quad b_4 \approx 3.8894 \,, \quad b_5 \approx -1.3512 \,, \quad b_6 \approx -2.4523 \,. \tag{4.121 b}$$

Finally, by using the scaling law $\mathcal{H} \approx \frac{N^2}{2}(1 - \log 2) + b_1 N^{3/2}$ for large N, the following rough estimate of the minimum value of the average MFPT $\bar{v}$ in (4.120) for the case of $N \gg 1$ circular traps of a common radius ε can be obtained:

$$\bar{v} \sim \frac{|\Omega|}{4\varepsilon D N}\left[1 - \frac{\varepsilon}{\pi}\log\varepsilon + \frac{\varepsilon N}{\pi}\left(\frac{1}{5} + \frac{4b_1}{\sqrt{N}}\right)\right] \,. \tag{4.122 a}$$

In terms of the trap surface area fraction f, given by $f = N\varepsilon^2/4$, (4.122 a) can be written equivalently as

$$\bar{v} \sim \frac{|\Omega|}{8D\sqrt{fN}}\left[1 - \frac{\sqrt{f/N}}{\pi}\log\left(\frac{4f}{N}\right) + \frac{2\sqrt{fN}}{\pi}\left(\frac{1}{5} + \frac{4b_1}{\sqrt{N}}\right)\right] \,. \tag{4.122 b}$$

Remarks: (Open Problems)

(1) Determine the relationship between the limiting results for large N and those that can be obtained by the dilute fraction limit of homogenization theory.

(2) Extend the analysis to other 3-D domains, by either determining detailed properties of the surface Green's

function either analytically or numerically. Devise a numerical method to compute the surface Green's function and to identify the regular part of the singularity structure.

(3) Extend the analysis to the case of a large sphere with reflecting boundary that contains a smaller interior sphere, for which the surface of the smaller sphere consists of many small pores. This narrow capture problem would involve naturally two small scales, and the results for the MFPT would (crudely) model the time taken for a viral particle that enters the cell to deposit its genetic material inside the cell nucleus.

5 Some Biharmonic Problems in Singular Perturbed Domains

In this section we first consider a few simple singularly perturbed biharmonic problems in the annulus $0 < \varepsilon < |x| < 1$ in $\mathbb{R}^2$ with $\varepsilon \to 0^+$. These model problems serve to illustrate the asymptotic methodology required to treat the linear and nonlinear biharmonic eigenvalue problems in perforated domains, and how the analysis differs from that of second-order elliptic problems in 2-D perforated domains considered previously in §3 and §4. We formulate a simple model problem as

$$\Delta^2 u = 0 \,, \quad x \in \Omega \backslash \Omega_\varepsilon \,, \tag{5.1 a}$$

$$u = f \,, \quad u_r = 0 \,, \quad \text{on} \quad r = 1 \,; \qquad u = u_r = 0 \,, \quad r = \varepsilon \,. \tag{5.1 b}$$

Here Ω is the unit disk centered at the origin and $\Omega_\varepsilon \equiv \{x \mid |x| \le \varepsilon\}$. Two choices for f are considered: **Case I:** $f = 1$. **Case II:** $f = \sin\theta$. We obtain an exact solution for each of these two cases, and then reconstruct them with a singular perturbation analysis. The analysis will show some novel features of singularly perturbed biharmonic BVP's.

For **Case I** where $f = 1$, the radially symmetric solution to (5.1) is a linear combination of $\{r^2, r^2 \log r, \log r, 1\}$. The solution to $\Delta^2 u = 0$, which satisfies the conditions on $r = 1$, has the form

$$u = A\left(r^2 - 1\right) + Br^2 \log r - (2A + B)\log r + 1 \,, \tag{5.2}$$

for any constants A and B. Upon imposing that $u = u_r = 0$ on $r = \varepsilon$, we get two equations for A and B

$$A = -\frac{B}{2}\left(1 - \frac{2\varepsilon^2 \log\varepsilon}{1 - \varepsilon^2}\right) , \qquad A\left(1 + 2\log\varepsilon - \varepsilon^2\right) + B\left(1 - \varepsilon^2\right)\log\varepsilon = 1 \,. \tag{5.3}$$

Upon substituting the first equation for A into the second, we obtain that B satisfies

$$-\frac{B}{2} - \frac{B\log\varepsilon}{1 - \varepsilon^2} + \frac{B\varepsilon^2 \log\varepsilon}{1 - \varepsilon^2} + \frac{2\varepsilon^2 B(\log\varepsilon)^2}{(1 - \varepsilon^2)^2} + B\log\varepsilon = \frac{1}{1 - \varepsilon^2} \,, \tag{5.4}$$

which reduces to $-B + 4\varepsilon^2(\log\varepsilon)^2 B \sim 2 + \mathcal{O}(\varepsilon^2)$. This determines B, and the first equation of (5.3) determines A. In this way, we get

$$B \sim -2 - 8\varepsilon^2 \left(\log\varepsilon\right)^2 \,, \qquad A \sim 1 + 4\varepsilon^2 \left(\log\varepsilon\right)^2 \,. \tag{5.5}$$

From (5.5) and (5.2), we obtain that a two-term expansion in the outer region $r \gg \mathcal{O}(\varepsilon)$ is

$$u \sim u_0(r) + \varepsilon^2 \left(\log\varepsilon\right)^2 u_1(r) + \mathcal{O}(\varepsilon^2 \log\varepsilon) \,, \tag{5.6 a}$$

where $u_0(r)$ and $u_1(r)$ are defined by

$$u_0(r) = r^2 - 2r^2 \log r \,, \qquad u_1 = 4\left(r^2 - 1\right) - 8r^2 \log r \,. \tag{5.6 b}$$

We emphasize that the leading-order outer solution $u_0(r)$ satisfies the point constraint $u_0(0) = 0$ and is not a C^2 smooth function. Hence, in the limit of small hole radius, the ε-dependent solution does not tend to the unperturbed solution in the absence of the hole. This unperturbed solution would have $B = 0$ and $A = 0$ in (5.2), and consequently $u \sim 1$ in the outer region. In fact, we note that $u_0(r)$ can be written as $u_0(r) = 1 - 16\pi G(r; 0)$, where

$$G(r; 0) = \frac{1}{8\pi}\left(r^2 \log r - \frac{r^2}{2} + \frac{1}{2}\right) \,, \tag{5.7}$$

is the biharmonic Green's function satisfying $\Delta^2 G = \delta(x)$ with $G = G_r = 0$ on $r = 1$.

Next, we show how to recover (5.6) from a matched asymptotic expansion analysis. In the outer region we expand the solution to (5.1) with $f = 1$ as

$$u \sim w_0 + \sigma w_1 + \cdots \,, \tag{5.8}$$

where $\sigma \ll 1$ is an unknown gauge function, and where w_0 satisfies the following problem with a point constraint:

$$\Delta^2 w_0 = 0 \,, \quad 0 < r < 1 \,; \qquad w_0(1) = 1 \,, \quad w_{0r}(1) = 0 \,, \quad w_0(0) = 0 \,. \tag{5.9}$$

Since $G(0; 0) = 1/(16\pi)$ from (5.7), the solution to (5.9) is $w_0 = 1 - 16\pi G(r; 0)$, which yields

$$w_0 = r^2 - 2r^2 \log r \,. \tag{5.10}$$

The problem for w_1 is

$$\Delta^2 w_1 = 0 \,, \quad 0 < r < 1 \,; \quad w_1(1) = w_{1r}(1) = 0 \,, \tag{5.11}$$

which has the following solution in terms of unknown coefficients α_1 and β_1:

$$w_1 = \alpha_1 \left(r^2 - 1\right) + \beta_1 r^2 \log r - (2\alpha_1 + \beta_1) \log r \,. \tag{5.12}$$

The behavior of w_1 as $r \to 0$, as found below by matching to the inner solution, will determine α_1 and β_1.

In the inner region we set $r = \varepsilon\rho$ and obtain from (5.10) that terms of order $\mathcal{O}(\varepsilon^2 \log \varepsilon)$ and $\mathcal{O}(\varepsilon^2)$ will be generated in the inner region. Therefore, this suggests that in the inner region we must expand the solution as

$$v(\rho) = u(\varepsilon\rho) = \left(\varepsilon^2 \log \varepsilon\right) v_0(\rho) + \varepsilon^2 v_1(\rho) + \cdots \,, \tag{5.13}$$

where v_0 and v_1 must satisfy $v_j(1) = v_{j\rho}(1) = 0$ for $j = 0, 1$. Therefore, we obtain for $j = 0, 1$ that

$$v_j = A_j \left(\rho^2 - 1\right) + B_j \rho^2 \log \rho - (2A_j + B_j) \log \rho \,. \tag{5.14}$$

We substitute (5.14) into (5.13) and write the resulting expression in terms of the outer variable $r = \varepsilon\rho$. A short calculation shows that the far-field behavior of (5.13) as $\rho \to \infty$, when written in the outer r variable, is

$$v \sim -(\log \varepsilon)^2 B_0 r^2 + (\log \varepsilon)\left[(A_0 - B_1) r^2 + B_0 r^2 \log r\right] + A_1 r^2 + B_1 r^2 \log r + (2A_0 + B_0)\,\varepsilon^2 (\log \varepsilon)^2 + \mathcal{O}(\varepsilon^2 \log \varepsilon) \,. \tag{5.15}$$

In contrast, the two-term outer solution from (5.8), (5.10), and (5.12), is

$$u \sim r^2 - 2r^2 \log r + \sigma \left[\alpha_1 \left(r^2 - 1 \right) + \beta_1 r^2 \log r - (2\alpha_1 + \beta_1) \log r \right] + \cdots . \tag{5.16}$$

Upon comparing (5.16) with (5.15), we conclude that

$$B_0 = 0 \,, \quad B_1 = A_0 \,, \quad A_1 = 1 \,, \quad B_1 = -2 \,, \quad \sigma = \varepsilon^2 \left(\log \varepsilon \right)^2 \,. \tag{5.17}$$

This leaves the unmatched constant term $-4\varepsilon^2(\log\varepsilon)^2$ on the right-hand side of (5.15). Consequently, it follows that the outer correction w_1 in (5.12) is bounded as $r \to 0$ and has the point constraint $w_1(0) = -4$. Consequently, $2\alpha_1 + \beta_1 = 0$ and $\alpha_1 = 4$ in (5.16). This gives $\beta_1 = -8$, and specifies the second-order outer correction term as

$$w_1 = 4 \left(r^2 - 1 \right) - 8r^2 \log r \,. \tag{5.18}$$

This expression reproduces that obtained in (5.6) from the perturbation of the exact solution.

The key feature in this model problem is that it is impossible to generate an inner solution that will match to an outer solution that has a prescribed value of $u_0(0) \neq 0$. The inner solution is a linear combination of $\{\rho^2, \rho^2 \log \rho, \log \rho, 1\}$. Upon setting the coefficients of the ρ^2 and $\rho^2 \log \rho$ term to zero, and even allowing for a logarithmic gauge function pre-multiplying the $\log \rho$ term, we would have an over-constrained problem in satisfying the two conditions on $\rho = 1$ and a prescribed matching condition at infinity. Thus, we must instead specify the point constraint $u_0(0) = 0$, so that the outer solution has a singularity of order $\mathcal{O}(r^2 \log r)$ as $r \to 0$. This model problem is closely related to the biharmonic nonlinear eigenvalue problem analyzed in §4.

Next, we consider **Case II** where $f = \sin\theta$ in (5.1). The solution to this model problem contains an infinite-order logarithmic expansion, which we show how to sum. The exact solution to (5.1) with $f = \sin\theta$ is a linear combination of $\{r^3, r\log r, r, r^{-1}\}\sin\theta$. Thus, the exact solution to (5.1), which satisfies the two conditions on $r = 1$, is

$$u = \left(Ar^3 + Br \log r + \left(-2A + \frac{1}{2} - \frac{B}{2} \right) r + \left(\frac{1}{2} + A + \frac{B}{2} \right) \frac{1}{r} \right) \sin\theta \,, \tag{5.19}$$

for any constants A and B. Then, by imposing that $u = u_r = 0$ on $r = \varepsilon$, we get two equations for A and B

$$A\varepsilon^3 + B\varepsilon \log \varepsilon + \left(-2A + \frac{1}{2} - \frac{B}{2} \right) \varepsilon + \left(\frac{1}{2} + A + \frac{B}{2} \right) \varepsilon^{-1} = 0 \,, \tag{5.20 a}$$

$$3A\varepsilon^2 + B + B \log \varepsilon + \left(-2A + \frac{1}{2} - \frac{B}{2} \right) - \left(\frac{1}{2} + A + \frac{B}{2} \right) \varepsilon^{-2} = 0 \,. \tag{5.20 b}$$

By comparing the $\mathcal{O}(\varepsilon^{-1})$ and $\mathcal{O}(\varepsilon^{-2})$ terms in (5.20), it is convenient to define κ by

$$\frac{1}{2} + A + \frac{B}{2} = \kappa\varepsilon^2 \,, \tag{5.21}$$

where κ is an $\mathcal{O}(1)$ constant to be found. Substituting (5.21) into (5.20), and neglecting the higher order $A\varepsilon^3$ and $3A\varepsilon^2$ terms in (5.20), we obtain the approximate system

$$B \log \varepsilon + \left(-2A + \frac{1}{2} - \frac{B}{2} \right) \approx -\kappa \,, \qquad B + B \log \varepsilon + \left(-2A + \frac{1}{2} - \frac{B}{2} \right) \approx \kappa \,. \tag{5.22}$$

By adding the two equations above to eliminate κ, we obtain that

$$B + 2B \log \varepsilon + (-4A + 1 - B) = 0 \,. \tag{5.23}$$

From (5.23), together with $A \sim -(1+B)/2$ from (5.21), we conclude that

$$B \sim \frac{3\nu}{2-\nu}\,, \qquad A = 1 - \frac{3}{2-\nu}\,, \quad \text{where} \quad \nu \equiv \frac{-1}{\log\left[\varepsilon e^{1/2}\right]}\,. \tag{5.24}$$

Finally, substituting (5.24) into (5.19), we obtain that the outer solution in $r \gg \mathcal{O}(\varepsilon)$ has the asymptotics

$$u \sim \left((1-\tilde{A})r^3 + \nu\tilde{A}r\log r + \tilde{A}r\right)\sin\theta\,, \tag{5.25 a}$$

where $\tilde{A}$ is defined by

$$\tilde{A} \equiv \frac{3}{2-\nu}\,, \qquad \nu \equiv \frac{-1}{\log\left[\varepsilon e^{1/2}\right]}\,. \tag{5.25 b}$$

We remark that (5.25) is an infinite-order logarithmic series approximation to the exact solution. However, it does not contain transcendentally small terms of algebraic order in ε as $\varepsilon \to 0$.

Next, we show how to recover (5.25) by formulating an appropriate singularity behavior near $r=0$, which has the effect of specifying both the singular and the regular part of a singularity structure.

In the inner region, with inner variable $\rho \equiv \varepsilon^{-1}r$, we look for an inner solution of the form $v_0(\rho)\sin\theta$ where v_0 has growth $\mathcal{O}(\rho\log\rho)$ as $\rho\to\infty$ and satisfies $v_0(1) = v_{0\rho}(1) = 0$. Upon multiplying this solution by $\varepsilon\nu C(\nu)$, where $C(\nu)$ is a constant with $C = \mathcal{O}(1)$ as $\nu \to 0$, we obtain that the inner solution has the form

$$v(\rho,\theta) = u(\varepsilon\rho,\theta) \sim \varepsilon\nu C(\nu)\left(\rho\log\rho - \frac{\rho}{2} + \frac{1}{2\rho}\right)\sin\theta\,. \tag{5.26}$$

Here $\nu \equiv -1/\log\left[\varepsilon e^{1/2}\right]$ and $C(\nu)$ is a function of ν to be found. The extra factor of ε in (5.26) is needed since the solution in the outer region is not algebraically large as $\varepsilon \to 0$. Now letting $\rho\to\infty$, and writing (5.26) in terms of the outer variable $r = \varepsilon\rho$, we obtain that the far-field form of (5.26) is

$$v \sim (C\nu r\log r + Cr)\sin\theta\,. \tag{5.27}$$

Therefore, the outer solution u_H to (5.1), which sums all the logarithmic terms in powers of ν, must satisfy

$$\Delta^2 u_H = 0\,, \quad 0<r<1\,; \qquad u_H = \sin\theta\,, \quad \partial_r u_H = 0\,, \quad \text{on} \quad r=1\,, \tag{5.28 a}$$

$$u_H = (C\nu r\log r + Cr)\sin\theta + o(r)\,, \quad \text{as} \quad r\to 0\,. \tag{5.28 b}$$

The singularity structure in (5.28 *b*) specifies both the strength of the singular term $C\nu r\log r\sin\theta$ in addition to the specific form $Cr\sin\theta$ for the regular part. As such, (5.28 *b*) provides an equation for the determination of C.

The solution to (5.28 *a*) is

$$u_H = \left(\alpha r^3 + \beta r\log r + \left(-2\alpha + \frac{1}{2} - \frac{\beta}{2}\right)r + \left(\frac{1}{2} + \alpha + \frac{\beta}{2}\right)\frac{1}{r}\right)\sin\theta\,, \tag{5.29}$$

while the singularity condition (5.28 *b*) yields the three equations

$$\beta = C\nu\,, \qquad -2\alpha + \frac{1}{2} - \frac{\beta}{2} = C\,, \qquad \frac{1}{2} + \alpha + \frac{\beta}{2} = 0\,, \tag{5.30}$$

for α, β, and C. We solve this system to obtain

$$\beta = C\nu\,, \qquad C = \frac{3}{2-\nu}\,, \qquad \alpha = 1 - C\,. \tag{5.31}$$

Upon substituting (5.31) into (5.29), and identifying $\tilde{A} = C$, we obtain that the resulting expression agrees exactly with the result (5.25) derived from the asymptotic expansion of the exact solution.

This simple model problem, whose solution contains an infinite-order logarithmic expansion, is closely related to the linear biharmonic eigenvalue problem that is studied below.

5.1 A Biharmonic Linear Eigenvalue Problem in a Perforated 2-D Domain

Next, we follow [**39**] and consider a singularly perturbed linear biharmonic eigenvalue problem in a two-dimensional domain Ω that is perforated by a small arbitrarily-shaped hole Ω_ε of "radius" ε such that $\Omega_\varepsilon \to x_0 \in \Omega$ as $\varepsilon \to 0$. The perturbed eigenvalue problem is formulated as

$$\Delta^2 u - \lambda u = 0\,, \quad x \in \Omega \backslash \Omega_\varepsilon\,; \qquad \int_{\Omega\backslash\Omega_\varepsilon} u^2\, dx = 1\,, \tag{5.32 a}$$

$$u = \partial_n u = 0\,, \quad x \in \partial\Omega\,; \qquad u = \partial_n u = 0\,, \quad x \in \partial\Omega_\varepsilon\,. \tag{5.32 b}$$

We will determine an asymptotic expansion for $\lambda(\varepsilon)$ as $\varepsilon \to 0$, with limiting behavior $\lambda(\varepsilon) \to \lambda_0$ as $\varepsilon \to 0$. This leading term λ_0, and its corresponding eigenfunction u_0, are an eigenpair of the following limiting problem with a point constraint, referred to as the punctured plate problem:

$$\Delta^2 u_0 - \lambda_0\, u_0 = 0\,, \quad x \in \Omega \setminus \{x_0\}\,; \qquad \int_\Omega u_0^2\, dx = 1\,, \tag{5.33 a}$$

$$u_0 = \partial_n u_0 = 0\,, \quad x \in \partial\Omega\,; \qquad u_0(x_0) = 0\,. \tag{5.33 b}$$

The key feature in this problem, as shared by the model problem in Case I of §2, is that we must introduce the point constraint $u_0(x_0) = 0$. Therefore, in the limit of small hole radius, the eigenvalue for the perforated eigenvalue problem (5.32) does not tend to an eigenvalue of the biharmonic eigenvalue problem in the domain without a hole. The limiting punctured plate eigenvalue problem (5.33) has a countably infinite set of eigenvalues with corresponding orthogonal eigenfunctions (cf. [**12**]), each with singular behavior $\mathcal{O}(|x - x_0|^2 \log|x - x_0|)$ as $x \to x_0$.

To solve the limiting problem (5.33) it is convenient to introduce the Green's function $G(x; x_0, \lambda_0)$ satisfying

$$\Delta^2 G - \lambda_0\, G = \delta(x)\,, \quad x \in \Omega \setminus \{x_0\}\,; \qquad G = \partial_n G = 0\,, \quad x \in \partial\Omega\,. \tag{5.34 a}$$

Then, $G(x; x_0, \lambda_0)$ can be decomposed in terms of its singular part and its C^2 smooth "regular" part $R(x; x_0, \lambda_0)$ as

$$G(x; x_0, \lambda_0) = \frac{1}{8\pi}\, |x - x_0|^2 \log|x - x_0| + R(x; x_0, \lambda_0)\,. \tag{5.34 b}$$

In terms of G, the solution to (5.33), up to a normalization factor, is simply $u_0 = G(x; x_0, \lambda_0)$, where λ_0 is a root of

$$R(x_0; x_0, \lambda_0) = 0\,. \tag{5.35}$$

In developing an asymptotic expansion for $\lambda(\varepsilon)$ below, we will consider only the simplest case for which λ_0 is a root of (5.35) of multiplicity one with $\nabla_x R(x; x_0, \lambda_0)|_{x=x_0} \neq 0$. The asymptotic methodology needed to treat this problem is similar to that of Case II of §2.

We remark that the degenerate case for which λ_0 is a root of (5.35) of multiplicity one with $\nabla_x R(x; x_0, \lambda_0)|_{x=x_0} = 0$ is discussed in detail in [**39**].

We expand the eigenvalue $\lambda(\varepsilon)$ of (5.32), together with the outer solution for this problem, as

$$\lambda(\varepsilon) = \lambda_0 + \sum_{k=1}^{\infty} \nu^k \lambda_k + \cdots , \qquad u = u_0 + \sum_{k=1}^{\infty} \nu^k u_k + \cdots , \qquad \nu \equiv \frac{-1}{\log \varepsilon} , \tag{5.36}$$

where $u_0 = G(x; x_0, \lambda_0)$. Upon substituting these expansions into (5.32), we obtain that u_1 and u_k for $k > 1$ satisfy

$$\Delta^2 u_1 - \lambda_0 u_1 = \lambda_1 u_0 , \quad x \in \Omega \setminus \{x_0\} ; \qquad u_1 = \partial_n u_1 = 0 , \quad x \in \partial\Omega ; \qquad \int_\Omega u_0 u_1 \, dx = 0 , \tag{5.37 a}$$

$$\Delta^2 u_k - \lambda_0 u_k = \lambda_k u_0 + \sum_{i=1}^{k-1} \lambda_i u_{k-i} , \quad x \in \Omega \setminus \{x_0\} ; \qquad u_k = \partial_n u_k = 0 , \quad x \in \partial\Omega , \tag{5.37 b}$$

with some normalization condition on u_k for $k > 1$. The singularity behaviors for u_k for $k \geq 1$ as $x \to x_0$, which are required for determining λ_k for $k \geq 1$, are derived below after matching u_k as $x \to x_0$ to the far-field behavior of certain inner solutions near the hole.

In the inner region, we let $y = \varepsilon^{-1}(x - x_0)$ and we introduce the canonical vector-valued inner solution ψ_c defined as the unique solution of

$$\Delta_y^2 \psi_c = 0 , \quad y \in \mathbb{R}^2 \setminus \Omega_0 ; \qquad \psi_c = \partial_n \psi_c = 0 , \quad y \in \partial\Omega_0 ; \qquad \psi_c \sim y \log |y| , \quad \text{as} \quad |y| \to \infty . \tag{5.38 a}$$

Here $\Omega_0 \equiv \varepsilon^{-1}\Omega_\varepsilon$. In terms of this solution, there exists a unique 2×2 matrix $\mathcal{M}$, which depends on the shape of the hole, such that

$$\psi_c \sim y \log |y| + \mathcal{M} y + o(1) , \quad \text{as} \quad |y| \to \infty . \tag{5.38 b}$$

For an arbitrarily-shaped subdomain Ω_0, the matrix $\mathcal{M}$ in (5.38 b) can be computed numerically from the integral equation method described in §5.1 of [**74**]. There are a few cases when $\mathcal{M}$ is known analytically. When Ω_0 is the unit disk, then the solution to (5.38) is

$$\psi_c = y \log |y| - \frac{y}{2} + \frac{y}{2|y|^2} , \tag{5.39}$$

so that $\mathcal{M} = -I/2$, where I is the identity matrix. In addition, when Ω_0 is an ellipse with semi-major axis a and semi-minor axis b, where $a > b$, and where the semi-major axis is inclined at an angle α to the horizontal coordinate $y_1 > 0$, it can be shown that the matrix entries of $\mathcal{M}$ are (see Appendix B of [**74**])

$$m_{11} = \frac{(b-a)\cos^2\alpha - b}{a+b} - \log\left(\frac{a+b}{2}\right) , \qquad m_{22} = \frac{(a-b)\cos^2\alpha - a}{a+b} - \log\left(\frac{a+b}{2}\right) , \tag{5.40 a}$$

$$m_{12} = m_{21} = -\frac{(a-b)\sin\alpha\cos\alpha}{a+b} . \tag{5.40 b}$$

In the inner region, we expand $u = \varepsilon\nu \sum_{k=0}^{\infty} \nu^k \psi_k$, where $\Delta_y^2 \psi_k = 0$. We take $\psi_k = a_k \cdot \psi_c$, where a_k is an unknown vector, $\cdot$ denotes dot product, and where the vector-valued function ψ_c satisfies (5.38). Thus, the inner expansion is

$$u = \varepsilon \nu \sum_{k=0}^{\infty} \nu^k a_k \cdot \psi_c \,. \tag{5.41}$$

Then, by using the far-field behavior (5.38 b) of ψ_c in (5.41), we write the resulting expression in terms of the outer variable $x - x_0 = \varepsilon y$ to get

$$u \sim a_0 \cdot (x - x_0) + \sum_{k=1}^{\infty} \nu^k \left[a_{k-1} \cdot (x - x_0) \log |x - x_0| + a_k \cdot (x - x_0) + a_{k-1} \cdot \mathcal{M}(x - x_0) \right] . \tag{5.42}$$

This gives the required singular behavior as $x \to x_0$ for each term in the outer expansion (5.36).

By comparing the leading-order terms in (5.36) and (5.42) for u, we obtain that $u_0 \sim a_0 \cdot (x - x_0)$ as $x \to x_0$. Since $u_0 = G(x; x_0, \lambda_0)$, we conclude from (5.34 b) that

$$a_0 = \nabla_x R(x; x_0, \lambda_0)|_{x=x_0} \,. \tag{5.43}$$

Then, by equating the $\mathcal{O}(\nu^k)$ terms in u in (5.36) and (5.42), we conclude that each u_k for $k \geq 1$ satisfies (5.37) subject to the singular behavior

$$u_k \sim a_{k-1} \cdot (x - x_0) \log |x - x_0| + \left[a_{k-1} \cdot \mathcal{M}(x - x_0) + a_k \cdot (x - x_0) \right] , \qquad \text{as} \quad x \to x_0 \,, \tag{5.44}$$

where a_0 is given in (5.43).

The problems (5.37) for $k \geq 1$, with singularity behavior (5.44), allows for the recursive determination of the unknown vectors a_k for $k \geq 1$, with a_0 as given in (5.43). In particular, with a known value for a_{k-1}, the singular behavior $u_k \sim a_{k-1} \cdot (x - x_0) \log |x - x_0|$ as $x \to x_0$ will determine λ_k from a solvability condition applied to (5.37). Then, the coefficient a_k in (5.44) is found from the regular part of the solution for u_k. Finally, u_k can be made unique by imposing a normalization condition.

The first step in this procedure is the calculation of λ_k. This is done with the following Lemma:

Lemma: *Let u_0, λ_0 be an eigenpair of (5.33) with multiplicity one, and assume that $\nabla_x R(x; x_0, \lambda_0)|_{x=x_0} \neq 0$. Then, a necessary condition for the problem*

$$\Delta^2 u_k - \lambda_0 u_k = \lambda_k u_0 + f(x) \,, \quad x \in \Omega \backslash \{x_0\} \,; \qquad u = \partial_n u = 0 \,, \quad x \in \partial\Omega \,, \tag{5.45 a}$$

$$u_k \sim a_{k-1} \cdot (x - x_0) \log |x - x_0| \,, \quad \text{as} \quad x \to x_0 \,, \tag{5.45 b}$$

to have a solution is that λ_k satisfies

$$\lambda_k \left(u_0, \, u_0 \right) = - \left(f, \, u_0 \right) + 4\pi a_{k-1} \cdot \nabla_x R_0 \,. \tag{5.46}$$

Here $\nabla_x R_0 \equiv \nabla_x R(x; x_0, \lambda_0)$, and we have defined the inner product $(g, \, h) \equiv \int_\Omega gh \, dx$.

The proof of this result follows by applying Green's identity to u_0 and u_k over the punctured domain $\Omega \backslash B_\delta$, where B_δ is a circular disk of radius $\delta \ll 1$ centered at x_0. This identity readily yields that

$$\lambda_k \int_{\Omega \backslash B_\delta} u_0^2 \, dx + \int_{\Omega \backslash B_\delta} f u_0 \, dx = \int_{\partial B_\delta} \left[u_0 \, \partial_n \left(\Delta u_1 \right) - \Delta u_1 \, \partial_n u_0 - u_1 \, \partial_n \left(\Delta u_0 \right) + \Delta u_0 \, \partial_n u_1 \right] \, ds \,. \tag{5.47}$$

Here ∂_n denotes the normal derivative directed inwards to B_δ, so that $\partial_n = -\partial_r$ where $r = |x - x_0|$. Next, we let

$\delta \to 0$, and use (5.34 *b*) for $u_0 = G(x; x_0, \lambda_0)$ together with (5.45 *b*) to calculate for $r \to 0$ that

$$u_k \sim (a_{k-1} \cdot e)\, r \log r \,, \quad \partial_r u_k \sim (a_{k-1} \cdot e) \left[\log r + 1\right] \,, \quad \Delta u_k \sim \frac{2}{r} \left(a_{k-1} \cdot e\right) \,, \quad \partial_r \left(\Delta u_k\right) \sim -\frac{2}{r^2} \left(a_{k-1} \cdot e\right) \,,$$

$$u_0 \sim (a_0 \cdot e)\, r + \frac{r^2}{8\pi} \log r \,, \quad \partial_r u_0 \sim (a_0 \cdot e) + \frac{r}{4\pi} \log r + \frac{r}{8\pi} \,, \quad \Delta u_0 \sim \frac{1}{2\pi} \log r + \frac{1}{2\pi} \,, \quad \partial_r \left(\Delta u_0\right) \sim \frac{1}{2\pi r} \,,$$

where $a_0 = \nabla_x R(x; x_0, \lambda_0)|_{x=x_0}$. Here we have defined e by $e \equiv (\cos\theta, \sin\theta)^T$. Upon substituting these limiting relations into (5.47), and then taking the limit $\delta \to 0$, we obtain that

$$\lambda_k \left(u_0,\, u_0\right) + \left(f,\, u_0\right) = \int_0^{2\pi} 4 \left(a_{k-1} \cdot e\right) \left(a_0 \cdot e\right) \, d\theta = 4\pi a_{k-1} \cdot a_0 = 4\pi a_{k-1} \cdot \nabla_x R_0 \,, \tag{5.49}$$

which completes the proof of the Lemma ■

By using the Lemma, we can calculate the coefficients λ_k in the asymptotic expansion of $\lambda(\varepsilon)$ from (5.37) and (5.44) to obtain the following main result:

Principal Result 5.1: *Let u_0, λ_0 be an eigenpair of (5.33) with multiplicity one, and assume that $\nabla_x R(x; x_0, \lambda_0)|_{x=x_0} \neq 0$. Then, the eigenvalue $\lambda(\varepsilon)$ for the perturbed problem (5.32) has the expansion*

$$\lambda(\varepsilon) \sim \lambda_0 + \nu \lambda_1 + \sum_{k=2}^{\infty} \nu^k \lambda_k \,, \qquad \nu \equiv \frac{-1}{\log \varepsilon} \,, \tag{5.50 a}$$

where λ_1 and λ_k for $k \geq 2$ are given by

$$\lambda_1 = 4\pi \frac{|\nabla_x R_0|^2}{(u_0,\, u_0)} \,, \qquad \lambda_k = \frac{1}{(u_0,\, u_0)} \left[4\pi a_{k-1} \cdot \nabla_x R_0 - \sum_{i=1}^{k-1} \lambda_i \left(u_{k-i},\, u_0\right) \right] \,, \tag{5.50 b}$$

and $\nabla_x R_0 \equiv \nabla_x R(x; x_0, \lambda_0)|_{x=x_0}$. In (5.50 b) the vectors a_k for $k \geq 1$, with $a_0 = \nabla_x R_0$, are determined recursively from the problems (5.37) and (5.44) for u_k for $k \geq 1$.

For the case of a circular hole of radius ε, then ψ_c satisfies (5.39) and $\mathcal{M} = -I/2$. For this special case we can conveniently replace ν and a_k in (5.50 *a*) and (5.50 *b*) with $\tilde{\nu} \equiv -1/\log\left(\varepsilon e^{1/2}\right)$ and b_k, respectively, where each u_k for $k \geq 1$, with $b_0 \equiv \nabla_x R_0$, satisfies (5.37) subject to the singularity behavior

$$u_k \sim b_{k-1} \cdot (x - x_0) \log|x - x_0| + b_k \cdot (x - x_0) \,, \quad \text{as} \quad x \to x_0 \,.$$

Finally, we remark that instead of evaluating the individual vector coefficients a_k for $k \geq 1$ needed in the Principal Result 5.1, it is possible to formulate a hybrid problem that effectively sums the infinite logarithmic expansion in (5.50 *a*). To do so, we write the inner solution in terms of an unknown vector $A = A(\nu)$ as

$$u = \varepsilon \nu A \cdot \psi_c(y) \,, \tag{5.51}$$

where $\psi_c(y)$ is the unique solution to (5.38). By using (5.38 *b*), the far-field behavior of this solution, as written in terms of the outer variable $x = x_0 + \varepsilon y$, is

$$u \sim A \cdot (x - x_0) + \nu A \cdot \left[(x - x_0) \log|x - x_0| + \mathcal{M}(x - x_0)\right] \,, \qquad \nu = \frac{-1}{\log \varepsilon} \,. \tag{5.52}$$

This expression gives the required singularity behavior for the outer solution accurate to within all logarithmic terms. In this way, the hybrid method for summing the infinite logarithmic expansion for $\lambda(\varepsilon)$ is to solve the following hybrid problem for $u^\star$, $\lambda^\star$, and the vector $A = A(\nu)$:

$$\Delta^2 u^\star - \lambda^\star u^\star = 0\,, \quad x \in \Omega \setminus \{x_0\}\,; \qquad u^\star = \partial_n u^\star = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega (u^\star)^2 \, dx = 1\,, \tag{5.53 a}$$

$$u \sim A \cdot (x - x_0) + \nu A \cdot \left[(x - x_0) \log|x - x_0| + \mathcal{M}(x - x_0)\right]\,, \qquad \nu = \frac{-1}{\log \varepsilon}\,. \tag{5.53 b}$$

Then, to within a negligible transcendentally small algebraic error term in ε, we have $\lambda(\varepsilon) \sim \lambda^\star$, as $\varepsilon \to 0$.

We now illustrate the theory by way of a specific example that can be solved analytically. Let Ω be the unit disk that contains an arbitrarily-shaped hole of "radius" ε centered at the origin. For $\varepsilon \to 0$, we look for an eigenfunction of the limiting problem (5.33) that has either a $\cos\theta$ or $\sin\theta$ dependence. A simple calculation shows that this type of solution to the limiting punctured plate eigenvalue problem (5.33) is given by

$$u_0 = c_0 \left(J_1(\eta_0 r) - \frac{J_1(\eta_0) I_1(\eta_0 r)}{I_1(\eta_0)} \right) \cos\theta + d_0 \left(J_1(\eta_0 r) - \frac{J_1(\eta_0) I_1(\eta_0 r)}{I_1(\eta_0)} \right) \sin\theta\,, \tag{5.54 a}$$

where $\eta_0 \equiv \lambda_0^{1/4}$ is taken to be the first positive root of the transcendental equation

$$J_1(\eta) I_1'(\eta) - J_1'(\eta) I_1(\eta) = 0\,. \tag{5.54 b}$$

Here c_0 and d_0 are arbitrary constants, while I_1 and J_1 denote Bessel functions in the standard notation. Therefore, the limiting eigenvalue problem has two independent eigenfunctions corresponding to the eigenvalue $\lambda_0 = \eta_0^4$.

For a non-circular hole, this degeneracy in the leading-order eigenpair is broken only at order $\mathcal{O}(\nu^2)$ in the expansion of the eigenvalue. To determine precisely how the eigenvalue is split by the asymmetry induced by the small arbitrarily-shaped hole, we will determine an infinite order expansion to the eigenvalue by using the hybrid formulation (5.53). This approach is more tractable analytically than evaluating all of the individual coefficients in the expansion of the eigenvalue as in the Principal Result 5.1.

From the hybrid formulation (5.53), $u^\star$, $\lambda^\star$ and $A = (A_1, A_2)^T$ satisfy (5.53 a) subject to the singular behavior (5.53 b) as $r \to 0$, which we write in expanded form as

$$u^\star \sim \left[A_1 \nu r \log r + A_1 r + \nu A_1 m_{11} r + \nu A_2 m_{21} r\right] \cos\theta + \left[A_2 \nu r \log r + A_2 r + \nu A_1 m_{12} r + \nu A_2 m_{22} r\right] \sin\theta\,. \tag{5.55}$$

Here m_{jk}, for $j,k = 1,2$, are the entries of the matrix $\mathcal{M}$ defined by (5.38 b). Since the required solution to (5.53 a) is a linear combination of $\{J_1(\eta r), Y_1(\eta r), I_1(\eta r), K_1(\eta r)\}(\cos\theta, \sin\theta)$, where $\eta \equiv (\lambda^\star)^{1/4}$, it can be written in terms of six unknown coefficients as

$$u^\star = \left[c_0 J_1(\eta r) + c_2 I_1(\eta r) + c_1 \left(Y_1(\eta r) + \frac{2}{\pi} K_1(\eta r) \right) \right] \cos\theta \\ + \left[d_0 J_1(\eta r) + d_2 I_1(\eta r) + d_1 \left(Y_1(\eta r) + \frac{2}{\pi} K_1(\eta r) \right) \right] \sin\theta\,. \tag{5.56}$$

Notice that this particular linear combination of Y_1 and K_1 eliminates the $1/r$ singularity in $u^\star$ as $r \to 0$.

From the well-known local behaviors of J_1, I_1, Y_1, and K_1, we calculate for $r \to 0$ that

$$Y_1(\eta r) + \frac{2}{\pi} K_1(\eta r) \sim \frac{2}{\pi} \eta r \log r + \frac{2\eta r}{\pi} \left[\log\left(\frac{\eta}{2}\right) + \gamma_e - \frac{1}{2} \right]\,, \qquad J_1(\eta r) \sim \frac{\eta r}{2}\,, \qquad I_1(\eta r) \sim \frac{\eta r}{2}\,, \tag{5.57}$$

where γ_e is Euler's constant. Then, we use (5.57) in (5.56) to obtain the local behavior of $u^\star$ as $r \to 0$. By comparing this local behavior of $u^\star$ with the required behavior in (5.55) we obtain upon examining the $\mathcal{O}(r\log r)$ term that

$$c_1 = \frac{A_1 \nu \pi}{2\eta}\,, \qquad d_1 = \frac{A_2 \nu\pi}{2\eta}\,. \tag{5.58 a}$$

Similarly, by comparing the $\mathcal{O}(r)$ terms in the local behavior of $u^\star$, we obtain

$$\frac{(c_0+c_2)}{2}\eta + A_1 b_{11} + A_2 b_{12} = 0\,, \qquad \frac{(d_0+d_2)}{2}\eta + A_1 b_{21} + A_2 b_{22} = 0\,, \tag{5.58 b}$$

where the coefficients b_{jk} for $j,k=1,2$ are defined by

$$b_{jj} = \nu\left(\log\left(\frac{\eta}{2}\right) + \gamma_e - \frac{1}{2}\right) - 1 - \nu m_{jj}\,, \quad j=1,2\,; \qquad b_{12} = -\nu m_{12}\,, \qquad b_{21} = -\nu m_{21}\,. \tag{5.58 c}$$

Finally, to ensure that $u^\star$ in (5.56) satisfies $u^\star = \partial_r u^\star = 0$ on $r=1$, we must impose that

$$\begin{pmatrix} c_0 \\ d_0 \end{pmatrix} J_1(\eta) + \begin{pmatrix} c_2 \\ d_2 \end{pmatrix} I_1(\eta) = -\frac{\nu\pi}{2\eta}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix}\left(Y_1(\eta) + \frac{2}{\pi}K_1(\eta)\right) = 0\,, \tag{5.58 d}$$

$$\begin{pmatrix} c_0 \\ d_0 \end{pmatrix} J_1'(\eta) + \begin{pmatrix} c_2 \\ d_2 \end{pmatrix} I_1'(\eta) = -\frac{\nu\pi}{2\eta}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix}\left(Y_1'(\eta) + \frac{2}{\pi}K_1'(\eta)\right) = 0\,. \tag{5.58 e}$$

The system (5.58) is a linear homogeneous system for the unknowns c_0, d_0, c_2, d_2, A_1, A_2, with eigenvalue parameter $\eta = (\lambda^\star)^{1/4}$. By using (5.58 *d*) and (5.58 *e*) to eliminate A_1 and A_2, a simple calculation shows that this system can be written as the equivalent 4×4 homogeneous system

$$\mathcal{A}\zeta = 0\,, \qquad \mathcal{A} \equiv \begin{pmatrix} b_{11}J_1(\eta) - \frac{\nu}{2\gamma_1} & b_{11}I_1(\eta) - \frac{\nu}{2\gamma_1} & b_{12}J_1(\eta) & b_{12}I_1(\eta) \\ J_1'(\eta) - \gamma_0 J_1(\eta) & I_1'(\eta) - \gamma_0 I_1(\eta) & 0 & 0 \\ b_{21}J_1(\eta) & b_{21}I_1(\eta) & b_{22}J_1(\eta) - \frac{\nu}{2\gamma_1} & b_{22}I_1(\eta) - \frac{\nu}{2\gamma_1} \\ 0 & 0 & J_1'(\eta) - \gamma_0 J_1(\eta) & I_1'(\eta) - \gamma_0 I_1(\eta) \end{pmatrix}, \tag{5.59 a}$$

where $\zeta \equiv (c_0, c_2, d_0, d_2)^T$ and $\nu = -1/\log\varepsilon$. In (5.59 *a*), γ_0 and γ_1 are defined by

$$\gamma_0 \equiv \left(\frac{Y_1'(\eta) + \frac{2}{\pi}K_1'(\eta)}{Y_1(\eta) + \frac{2}{\pi}K_1(\eta)}\right), \qquad \gamma_1 \equiv \frac{2}{\pi}\left[Y_1(\eta) + \frac{2}{\pi}K_1(\eta)\right]^{-1}\,. \tag{5.59 b}$$

In (5.59 *a*) the coefficients b_{jk}, for $j,k=1,2$, are defined in (5.58 *c*).

For the special case of a circular hole of radius ε, so that $m_{12} = m_{21} = 0$ and $m_{11} = m_{22} = -1/2$, then $b_{12} = b_{21}$ and $b_{11} = b_{22} = b_c \equiv \nu(\log(\eta/2) + \gamma_e - 1/2) - 1 + \nu/2$. For this special case, where the eigenfunction degeneracy is not broken, the matrix $\mathcal{A}$ can be written in block diagonal form and there are two independent vectors $\zeta_1 = (c_0, c_2, 0, 0)^T$ and $\zeta_2 = (0, 0, d_0, d_2)^T$ for the common eigenvalue $\lambda^\star = \eta^4$, where η is the first positive root of

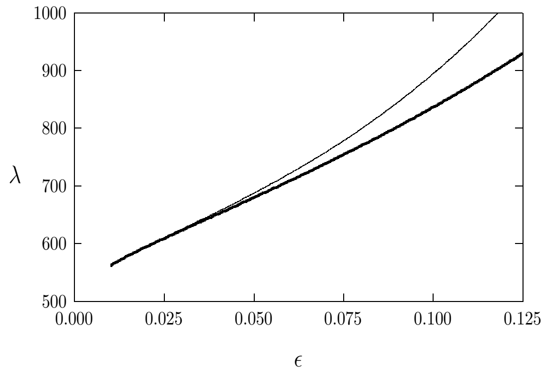
$$J_1(\eta)I_1'(\eta) - J_1'(\eta)I_1(\eta) = \frac{\nu}{2b_c\gamma_1}\left[I_1'(\eta) - J_1'(\eta) - \gamma_0\left(I_1(\eta) - J_1(\eta)\right)\right]\,. \tag{5.60}$$

For a circular hole of radius ε, in Fig. 9(a) we compare the asymptotic approximation $\lambda^\star$ versus ε, as obtained from (5.60), with the exact result for $\lambda(\varepsilon)$ as obtained by requiring that the solution

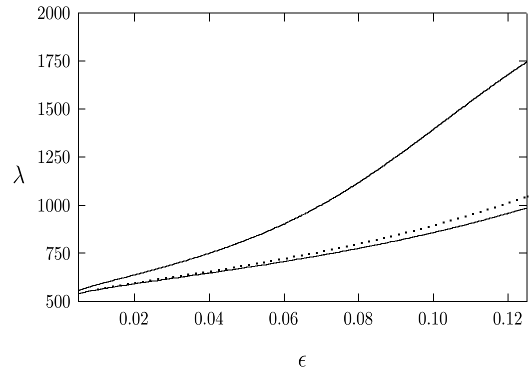
$$u = \left[c_0 J_1(\eta r) + c_2 I_1(\eta r) + c_3 K_1(\eta r) + c_4 Y_1(\eta r)\right]\cos\theta \tag{5.61}$$

to (5.32) satisfy the four conditions $u = u_r = 0$ on $r=\varepsilon$ and $r=1$. As seen from this figure, the asymptotic and full numerical results agree rather well on the range $0<\varepsilon<0.1$.

Next, consider an elliptical-shaped hole $x_1^2/a^2 + x_2^2/b^2 = \varepsilon^2$, for which the matrix entries of $\mathcal{M}$ are given in (5.40)



(a) Circular-shaped hole of radius ε



(b) Elliptical-shaped hole of semi-axes 2ε and $\varepsilon/2$

FIGURE 9. Left figure: For the annulus $\varepsilon < |x| < 1$, the asymptotic approximation $\lambda^\star$ (solid curve), as obtained from (5.60), is compared with the exact solution $\lambda(\varepsilon)$ (heavy solid curve), as obtained by requiring that (5.61) satisfy $u = u_r = 0$ on $r = \varepsilon$ and $r = 1$. Right figure: for the elliptical-shaped hole $x_1^2/4 + 4x_2^2 = \varepsilon^2$ of area $\pi\varepsilon^2$, the asymptotic approximations $\lambda_\pm = \eta_\pm^4$ (solid curves) are plotted versus ε, where $\eta_\pm$ are the first two roots of $\det(\mathcal{A}) = 0$ with $\mathcal{A}$ is defined in (5.59). The dotted curve is the asymptotic approximation $\lambda^\star$, as computed from (5.60), corresponding to the eigenvalue of multiplicity two for the case of a circular hole of the same area $\pi\varepsilon^2$.

with inclination angle $\alpha = 0$. For this example, when ε is small there are two nearby roots $\eta_\pm$ to $\det(\mathcal{A}) = 0$, where $\mathcal{A}$ is defined in (5.59), which have the common limiting behavior $\eta_\pm \to \eta_{00}$ as $\nu \to 0$. Here η_{00} is the first positive root of $J_1(\eta)I_1'(\eta) - J_1'(\eta)I_1(\eta) = 0$. In Fig. 9(b) we plot the two curves $\lambda_\pm = \eta_\pm^4$ versus ε for an elliptical-shaped hole with semi-axes $a = 2$ and $b = 1/2$. This example clearly shows how the asymmetry of the hole breaks the degeneracy of the eigenvalue of multiplicity two for the limiting problem (5.33), and leads to the creation of two closely-spaced simple eigenvalues for the perturbed problem (5.32).

6 Pattern Formation via Reaction-Diffusion Systems in 2-D Domains

Localized spatio-temporal patterns consisting of spots or clusters of spots have been observed in many physical and chemical experiments. Such localized patterns can exhibit a variety of dynamical behaviors and instabilities including slow spot drift, temporal oscillations of spots, spot annihilation, and spot self-replication. Physical experiments where some of this phenomena has been observed include the ferrocyanide-iodate-sulphite reaction (cf. [**44**]), the chloride-dioxide-malonic acid reaction (cf. [**21**]), and certain semiconductor gas discharge systems.

Numerical simulations of certain singularly perturbed two-component reaction-diffusion systems with very simple kinetics, such as the Gray-Scott model, have shown the occurrence of very complex spatio-temporal localized patterns consisting of either spots, stripes, or space-filling curves in a two-dimensional domain (cf. [**52**]). Some of these reduced two-component reaction-diffusion systems model, at least qualitatively, the more complex chemically interacting systems of the experimental studies of [**44**] and [**21**]. A survey of experimental and theoretical studies, through reaction-diffusion modeling, of localized spot patterns in various physical or chemical contexts is given in [**76**].

Mathematically, a spot pattern for a reaction-diffusion system in a multi-dimensional domain Ω is a spatial pattern where at least one of the solution components is highly localized near certain discrete points in Ω that can evolve dynamically in time. For certain singularly perturbed two-component reaction-diffusion models in one space dimension, such as the Gray-Scott and Gierer-Meinhardt models, there has been considerable analytical progress in understanding both the dynamics and the various types of instabilities of spike patterns, including self-replicating instabilities. In contrast, in a two-dimensional spatial domain there are relatively few studies characterizing spot dynamics and stability. For a detailed literature survey, see [**37**] and [**16**].

In this section we study a class of nonlinear reaction-diffusion problems with localized spot patterns in a two-dimensional domain, An example of such a problem is the Schnakenburg reaction-diffusion model, studied in [**37**], formulated as

$$v_t = \varepsilon^2 \triangle v - v + uv^2 \,, \qquad \varepsilon^2 u_t = D \triangle u + a - \varepsilon^{-2} uv^2 \,, \quad x \in \Omega \,; \qquad \partial_n u = \partial_n v = 0 \,, \quad x \in \partial\Omega \,. \tag{6.1}$$

Here $0 < \varepsilon \ll 1$, $D > 0$, and $a > 0$, are parameters.

We now construct a quasi steady-state solution to (6.1) with K localized spots. Such a solution is characterized by the concentration of v as $\varepsilon \to 0$ to the vicinity of K distinct locations $x_1, \ldots, x_N$ in Ω. We assume that the distance between any two spots is $\mathcal{O}(1)$ as $\varepsilon \to 0$. In the inner region near the j^{th} spot we introduce the new variables

$$u = \frac{1}{\sqrt{D}} \mathcal{U}_j \,, \qquad v = \sqrt{D} \mathcal{V}_j \,, \qquad y = \varepsilon^{-1}(x - x_j) \,. \tag{6.2}$$

In the inner region, we look for a leading-order radially symmetric solution of the form $\mathcal{U}_j \sim U_j(\rho)$ and $\mathcal{V}_j \sim V_j(\rho)$ with $\rho = |y|$. Thus, for each $j = 1, \ldots, K$, we have that U_j and V_j, with primes denoting derivatives in ρ, satisfy

$$V_j'' + \frac{1}{\rho} V_j' - V_j + U_j V_j^2 = 0 \,; \quad U_j'' + \frac{1}{\rho} U_j' - U_j V_j^2 = 0 \,, \quad 0 < \rho < \infty \,, \tag{6.3 a}$$

$$U_j'(0) = V_j'(0) = 0 \,; \quad V_j \to 0 \,, \quad U_j \sim S_j \log \rho + \chi(S_j) \quad \text{as} \quad \rho \to \infty \,. \tag{6.3 b}$$

The local variable V_j decays exponentially as $\rho \to \infty$. In contrast, the far-field logarithmic behavior for U_j in (6.3 b) is similar to that in (3.15) for the case where the inner problem is Laplace's equation. We emphasize that the nonlinear function $\chi = \chi(S_j)$ in (6.3 b) must be computed numerically from the solution to (6.3) as a function of the source strength $S_j > 0$.

Next, we determine the source strengths $S_1, \ldots, S_N$ by matching the far-field behavior of U_j to an outer solution for u valid away from $\mathcal{O}(\varepsilon)$ distances from x_j. Firstly, upon writing the far-field condition for U_j in (6.3 b) in terms of outer variables, we obtain from the matching condition that the outer solution for u must have the local behavior

$$u \sim \frac{1}{\sqrt{D}} \left[S_j \log|x - x_j| + \frac{S_j}{\nu} + \chi(S_j) \right] \,, \quad x \to x_j \,, \tag{6.4}$$

for $j = 1, \ldots, N$, where $\nu \equiv -1/\log \varepsilon$. Secondly, in the outer region, v is exponentially small, and from (6.2) and (6.3 b) we get

$$\varepsilon^{-2} uv^2 \to \frac{2\pi\sqrt{D}}{\varepsilon^2} \left(\varepsilon^2 \int_0^\infty \rho U_j V_j^2 \, d\rho \right) \delta(x - x_j) = 2\pi \sqrt{D} S_j \delta(x - x_j) \,. \tag{6.5}$$

Therefore, from (6.1), the outer steady-state solution for u satisfies

$$\Delta u = -\frac{a}{D} + \frac{2\pi}{\sqrt{D}} \sum_{j=1}^{K} S_j \, \delta(x - x_j) \,, \quad x \in \Omega \,; \qquad \partial_n u = 0 \,, \quad x \in \partial\Omega \,, \tag{6.6 a}$$

$$u \sim \frac{1}{\sqrt{D}} \left[S_j \log|x - x_j| + \chi(S_j) + \frac{S_j}{\nu} \right] \quad \text{as} \quad x \to x_j \,, \quad j = 1, \ldots, K \,, \tag{6.6 b}$$

where $\nu \equiv -1/\log\varepsilon$. We again observe that the singularity behavior in (6.6 b) specifies both the singular and regular parts of a Coulomb singularity. As such, each singularity behavior provides one equation for the determination of an algebraic system for the source strengths $S_1, \ldots, S_N$.

To solve this problem, we first note that the Divergence theorem enforces that $2\pi \sum_{j=1}^{K} S_j = a|\Omega|/\sqrt{D}$, where $|\Omega|$ is the area of Ω. The solution to (6.6) then can be represented in terms of the Neumann Green's function G_N of (3.55) by

$$u(x) = -\frac{2\pi}{\sqrt{D}} \left(\sum_{i=1}^{K} S_i G_N(x; x_i) + \chi \right) . \tag{6.7}$$

Here χ is a constant to be found. By expanding (6.7) as $x \to x_j$, and comparing the resulting expression with the required singularity behavior in (6.6 b), we obtain for each $j = 1, \ldots, K$ that

$$S_j \log|x - x_j| - 2\pi S_j R_N(x_j; x_j) - 2\pi\chi - 2\pi \sum_{\substack{i=1 \\ i \neq j}}^{K} S_i G_N(x_j; x_i) \sim S_j \log|x - x_j| + \chi(S_j) + \frac{S_j}{\nu} . \tag{6.8}$$

These matching conditions gives K equations relating $S_1, \ldots, S_N$ and χ. We summarize our construction as follows:

Principal Result 6.1: *For given spot locations x_j for $j = 1, \ldots, K$, let S_j for $j = 1, \ldots, K$ and χ satisfy the nonlinear algebraic system*

$$S_j + 2\pi\nu \left(S_j R_{Njj} + \sum_{\substack{i=1 \\ i \neq j}}^{K} S_i G_{Nji} \right) + \nu\chi(S_j) = -2\pi\nu\chi \,; \qquad \sum_{j=1}^{K} S_j = \frac{a|\Omega|}{2\pi\sqrt{D}} . \tag{6.9}$$

Here $\nu \equiv -1/\log\varepsilon$ with $G_{Nji} \equiv G_N(x_j; x_i)$ and $R_{Njj} \equiv R_N(x_j; x_j)$, where G_N is the Neumann Green's function of (3.55) with regular part R_N. The nonlinear term $\chi(S_j)$ in (6.9) is as given in (6.3 b). Then, for $\varepsilon \to 0$, the outer solution for a K-spot quasi steady-state solution of (6.1) is given by (6.7), and the leading-order inner solutions are given by $u \sim D^{-1/2} U_j$ and $v \sim \sqrt{D} V_j$, where U_j and V_j is the solution to the core problem (6.3).

We emphasize that the system (6.9) contains all of the logarithmic correction terms of order $\mathcal{O}(\nu^k)$ for any k that are required in the construction of the quasi steady-state solution. Hence, we say that (6.9) has 'summed' all of the logarithmic terms in powers of ν for the source strengths $S_1, \ldots, S_N$. The key difference here between this nonlinear problem and the linear problem of §3 is that the source strengths now satisfy a nonlinear algebraic system of equations.

A detailed study of (6.9) and other aspects of localized pattern formation, including self-replicating spot patterns, is studied in [**37**].

In particular, we can proceed as in §2 of [**37**] to derive an ODE system for the slow evolution of the spots x_j for

$j = 1, \ldots, K$. In the inner region near $x = x_j$ we expand the solution to (6.1) as

$$u = \frac{1}{\sqrt{D}} \left(U_j(\rho) + \varepsilon U_{1j}(y_j) + \cdots \right) , \qquad v = \sqrt{D} \left(V_j(\rho) + \varepsilon V_{1j}(y_j) + \cdots \right) , \qquad y_j = \varepsilon^{-1} \left[x - x_j(\tau) \right] , \quad \tau = \varepsilon^2 t \, . \tag{6.10}$$

Here $U_j(\rho)$ and $V_j(\rho)$, with $\rho = |y_j|$, are the radial symmetric solutions of the core problem (6.3). We then substitute (6.10) into (6.1) and collect terms of order $\mathcal{O}(\varepsilon)$ to derive that V_{1j} and U_{1j} for each $j = 1, \ldots, K$ satisfies

$$\Delta_{y_j} W_{1j} + \mathcal{M}_j W_{1j} = f_j \, , \qquad y_j \in \mathbb{R}^2 \, , \tag{6.11 a}$$

where $y_j = \rho e_\theta$, and the vectors W_{1j}, f_j, e_θ and the 2×2 matrices $\mathcal{M}_j$ are defined by

$$W_{1j} \equiv \begin{pmatrix} V_{1j} \\ U_{1j} \end{pmatrix} , \qquad f \equiv \begin{pmatrix} -V_j^{\prime} x_j^{\prime} {\cdot} e_\theta \\ 0 \end{pmatrix} , \qquad e_\theta \equiv \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} , \qquad \mathcal{M}_j \equiv \begin{pmatrix} -1 + 2U_j V_j & V_j^2 \\ -2U_j V_j & -V_j^2 \end{pmatrix} . \tag{6.11 b}$$

The determination of a far-field condition for W_{1j} is derived by performing a higher order matching of the outer and inner solutions. In this way, we obtain that the solution to (6.11) must satisfy

$$W_{1j} \sim \begin{pmatrix} 0 \\ \alpha_j {\cdot} y_j \end{pmatrix} \quad \text{as} \quad y_j \to \infty \, , \qquad \alpha_j \equiv -2\pi S_j \nabla R(x_j; x_j) - 2\pi \sum_{\substack{j=1 \\ j \neq i}}^{N} S_i \nabla G(x_j; x_i) \, . \tag{6.12}$$

The problem (6.11) subject to (6.12) determines $x_j^\prime$ in terms of the vector α_j. In this way, we obtain the following main result for the dynamics of a K-spot quasi-equilibrium solution was obtained in [**37**].

<u>**Principal Result 6.2**</u>: *For $\varepsilon \to 0$ the slow dynamics of a collection $x_1, \ldots, x_K$ of spots satisfies the differential-algebraic system (DAE),*

$$x_j^\prime \sim -2\pi \varepsilon^2 \gamma(S_j) \left(S_j \nabla R(x_j; x_j) + \sum_{\substack{j=1 \\ j \neq i}}^{N} S_i \nabla G(x_j; x_i) \right) , \qquad j = 1, \ldots, K \, . \tag{6.13}$$

Here the source strengths S_j, for $j = 1, \ldots, K$, are determined in terms of $x_1, \ldots, x_K$ by the nonlinear algebraic system (6.9). The function $\gamma(S_j)$ is a certain positive function determined in terms of a solvability condition.

Next, we study the stability of the quasi-equilibrium one-spot solution constructed above to instabilities occurring on a fast $\mathcal{O}(1)$ time-scale. Since the speed of the slow drift of the spots in (6.13) is $\mathcal{O}(\varepsilon^2) \ll 1$, in our stability analysis we will assume that the spot is asymptotically stationary. We begin the stability analysis by letting u_e and v_e denote the quasi-equilibrium solution, and we introduce the perturbation

$$u = u_e + \mathrm{e}^{\lambda t} \eta \, , \qquad v = v_e + \mathrm{e}^{\lambda t} \phi \, . \tag{6.14}$$

By substituting (6.14) into (6.1) and linearizing, we obtain the following eigenvalue problem for ϕ and η:

$$\varepsilon^2 \Delta\phi - \phi + 2u_e v_e \phi + v_e^2 \eta = \lambda\phi \, , \quad D\Delta\eta - 2\varepsilon^{-2} u_e v_e \phi - \varepsilon^{-2} v_e^2 \eta = \varepsilon^2 \lambda \eta \, , \quad x \in \Omega \, ; \quad \partial_n \phi = \partial_n \eta = 0 \, , \quad x \in \partial\Omega \, . \tag{6.15}$$

In the inner region near x_0 we look for an $\mathcal{O}(1)$ time-scale instability associated with the local angular integer mode m by introducing the new variables $N(\rho)$ and $\Phi(\rho)$ by

$$\eta = \frac{1}{D} e^{im\theta} N(\rho) \, , \qquad \phi = e^{im\theta} \Phi(\rho) \, , \qquad \rho = |y| \, , \qquad y = \varepsilon^{-1}(x - x_0) \, , \tag{6.16}$$

where $y^t = \rho(\cos\theta, \sin\theta)$. Substituting (6.16) into (6.15), and by using $u_e \sim D^{-1/2} U(\rho)$ and $v_e \sim \sqrt{D} V(\rho)$, where U

m	Σ_m
2	4.303
3	5.439
4	6.143
5	6.403
6	6.517

Table 6. Numerical results computed from (6.17) for the threshold values of S, denoted by Σ_m, as a function of the integer angular mode m where an instability first occurs for the core problem (6.3) as S increases.

and V satisfy the core problem (6.3), we obtain the following radially symmetric eigenvalue problem:

$$\mathcal{L}_m\Phi - \Phi + 2UV\Phi + V^2N = \lambda\Phi\,, \qquad \mathcal{L}_mN - 2UV\Phi - V^2N = 0\,, \qquad 0 \leq \rho < \infty\,. \tag{6.17}$$

Here $\mathcal{L}_m\Phi \equiv \partial_{\rho\rho}\Phi + \rho^{-1}\partial_\rho\Phi - m^2\rho^{-2}\Phi$. We impose the usual regularity condition for Φ and N at $\rho = 0$. As we show below, the appropriate far-field boundary conditions for (6.17) as $\rho \to \infty$ depends on whether $m = 0$ or $m \geq 2$.

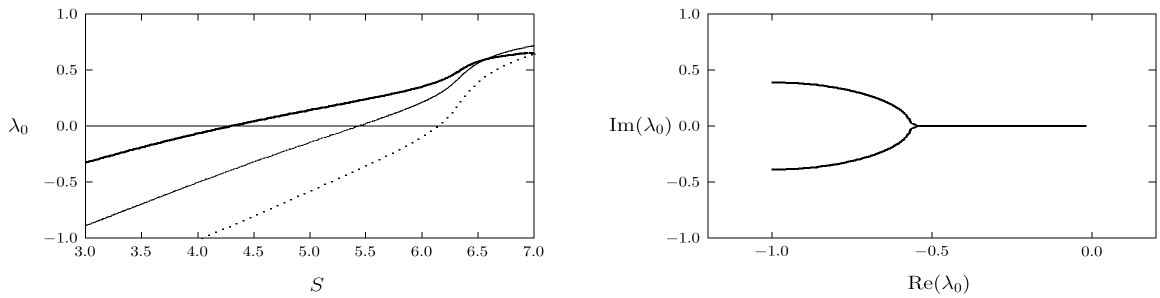
The eigenvalue problem (6.17) does not appear to be amenable to analysis, and thus we solve it numerically for various integer values of m. We denote λ_0 to be the eigenvalue of (6.17) with the largest real part. Since U and V depend on S from (6.3), we have implicitly that $\lambda_0 = \lambda_0(S, m)$. To determine the onset of any instabilities, we compute any threshold values $S = \Sigma_m$ where $\text{Re}(\lambda_0(\Sigma_m, m)) = 0$. In our computations, we only consider $m = 0, 2, 3, 4, \ldots$, since $\lambda_0 = 0$ for any value of S for the translational mode $m = 1$. A higher order perturbation analysis for the $m = 1$ mode generates only weak instabilities occurring on an asymptotically long $\mathcal{O}(\varepsilon^{-2})$ time-scale. Any such instabilities are reflected in instabilities in the ODE (6.13).

When $m \geq 2$ we can impose the asymptotic decay conditions that Φ decays exponentially as $\rho \to \infty$ while $N \sim \mathcal{O}(\rho^{-m}) \to 0$ as $\rho \to \infty$. With these conditions (6.17) is discretized with centered differences on a large but finite domain. We then determine $\lambda_0(S, m)$ by computing the eigenvalues of a matrix eigenvalue problem. For $m \geq 2$ our computations show that $\lambda_0(S, m)$ is real and that $\lambda_0(S, m) > 0$ when $S > \Sigma_m$. The threshold value Σ_m is tabulated in Table 6 for $m = 2, \ldots, 6$. In our computations we took 300 meshpoints on the interval $0 \leq \rho < 20$. To the number of significant digits shown in Table 6, the results there are insensitive to increasing either the domain length or the number of grid points. It follows from Table 6 that the smallest value of S where an instability is triggered occurs for the "peanut-splitting" instability $m = 2$ at the threshold value $S = \Sigma_2 \approx 4.3$. In Fig. 10(a) we plot $\lambda_0(S, m)$ as a function of S for $m = 2$, $m = 3$ and $m = 4$.

By extending this result to the K-spot case, the following result characterizing spot-splitting was obtained in [**37**].

Spot-Splitting Criterion: *Let $D = \mathcal{O}(1)$ and $\varepsilon \to 0$ and consider a K-spot quasi-equilibrium solution to (6.1). Let S_j for $j = 1, \ldots, K$, satisfy the nonlinear algebraic system (6.9) when $K > 1$. For $K \geq 1$ the quasi-equilibrium solution is stable with respect to the other local angular modes $m = 2, 3, 4, \ldots$ provided that $S_j < \Sigma_2 \approx 4.303$ for all $j = 1, \ldots, K$. The J^{th} spot will become unstable to the $m = 2$ mode if S_J exceeds the threshold value Σ_2. This peanut-splitting instability from the linearized problem is found to initiate a nonlinear spot self-replication process.*

Numerical confirmation of this theory was shown in [**37**], and will be illustrated in class.



(a) λ_0 vs. S for $m = 2, 3, 4$ (b) $\mathrm{Im}(\lambda_0)$ and $\mathrm{Re}(\lambda_0)$ for $m = 0$

FIGURE 10. Left figure: Plot of the largest (real) eigenvalue $\lambda_0(S, m)$ of (6.17) vs. S for $m = 2$ (heavy solid), $m = 3$ (solid), and $m = 4$ (dotted). Right figure: Plot in the complex plane of the path of the eigenvalue $\lambda_0(S, 0)$ of largest real part of (6.17) with $m = 0$ and $2.8 < S < 7.5$. For $S < 2.8$, $\lambda_0 \approx -1.0$ and arises from the discretization of the continuous spectrum (not shown). For $2.8 < S < 4.98$, $\lambda_0(S, 0)$ occurs as a complex conjugate pair which monotonically approaches the real axis as S increases. This pair merges onto the real axis at $S \approx 4.79$. As S increases further, $\lambda_0(S, 0)$ remains real but negative.

7 Conclusion

In these notes we have surveyed the development and application of a singular perturbation methodology for solving linear and nonlinear PDE models in two- or three-dimensional domains that have small inclusions or obstructions, or localized regions where the solution changes significantly. Although this strong localized perturbation theory has has been illustrated on some specific problems, the framework of the methodology applies rather widely. We have also listed a few specific open problems that warrant further study. Moreover, we emphasize that the approach of applying ideas from strong localized perturbation theory to the study of reaction-diffusion theory patterns in cell signalling or in chemical physics is largely open-ended with many interesting avenues for research.

Appendix A Solutions to the Problems in §2

Solution to Problem 2.1:

We now use the method of matched asymptotic expansions to derive a two-term expansion for the principal eigenvalue $\lambda(\varepsilon)$ of (2.17) as $\varepsilon \to 0$. For the problem with no traps, $\lambda_0 = 0$ and $u_0 = |\Omega|^{-1/2}$ is the unperturbed eigenfunction, where $|\Omega|$ denotes the volume of Ω. We expand the principal eigenvalue for (2.17) as

$$\lambda = \varepsilon\lambda_1 + \varepsilon^2\lambda_2 + \cdots . \tag{A.1}$$

In the outer region away from an $\mathcal{O}(\varepsilon)$ neighborhood of x_j, we expand the outer solution as

$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots . \tag{A.2}$$

Upon substituting (A.1) and (A.2) into (2.17 a) and (2.17 b), we obtain that u_1 and u_2 satisfy

$$\Delta u_1 = -\lambda_1 u_0 \,, \quad x \in \Omega\backslash\{x_1, \ldots x_N\} \,; \qquad \partial_n u_1 = 0 \,, \quad x \in \partial\Omega \,; \qquad \int_\Omega u_1 \, dx = 0 \,. \tag{A.3}$$

$$\Delta u_2 = -\lambda_2 u_0 - \lambda_1 u_1 \,, \quad x \in \Omega\backslash\{x_1, \ldots x_N\} \,; \qquad \partial_n u_2 = 0 \,, \quad x \in \partial\Omega \,; \qquad \int_\Omega u_2 \, dx = -\frac{|\Omega|^{1/2}}{2} \int_\Omega u_1^2 \, dx \,. \tag{A.4}$$

The matching of u_1 and u_2 to inner solutions defined in an $\mathcal{O}(\varepsilon)$ neighborhood of each trap will yield singularity conditions for u_1 and u_2 as $x \to x_j$ for $j = 1, \ldots, N$. .

In the inner region near the j^{th} trap we introduce the local variables y and $w(y)$ by

$$y = \varepsilon^{-1}(x - x_j)\,, \qquad w(y) = u(x_j + \varepsilon y, \varepsilon)\,. \tag{A.5}$$

Upon substituting (A.5) into (2.17 a) and (2.17 c), we obtain that $\Delta_y w = -\varepsilon^2 \lambda w$, where Δ_y denotes the Laplacian in the y variable. We expand the inner solution as

$$w = w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \cdots\,, \tag{A.6}$$

and then use $\lambda = \mathcal{O}(\varepsilon)$ to obtain the following inner problems for $k = 0, 1, 2$:

$$\Delta_y w_k = 0\,, \quad y \notin \Omega_j\,; \qquad w_k = 0\,, \quad y \in \partial\Omega_j\,. \tag{A.7}$$

Here Ω_j denotes an $\mathcal{O}(\varepsilon^{-1})$ magnification of Ω_{ε_j} so that $\Omega_j = \varepsilon^{-1}\Omega_{\varepsilon_j}$. The appropriate far-field boundary condition for (A.7) is determined by matching w to the outer asymptotic expansion of the eigenfunction.

The matching condition is that the near-field behavior of the outer eigenfunction as $x \to x_j$ must agree asymptotically with the far-field behavior of the inner eigenfunction as $|y| = \varepsilon^{-1}|x - x_j| \to \infty$, so that

$$u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots \sim w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + \cdots\,. \tag{A.8}$$

Since $u_0 = |\Omega|^{-1/2}$, the first matching condition is that $w_0 \sim |\Omega|^{-1/2}$ as $|y| \to \infty$. We then introduce w_c by

$$w_0 = \frac{1}{|\Omega|^{1/2}}\left(1 - w_c\right)\,, \tag{A.9}$$

so that from (A.7) with $k = 0$, we get that w_c satisfies

$$\Delta_y w_c = 0\,, \quad y \notin \Omega_j\,; \qquad w_c = 1\,, \quad y \in \partial\Omega_j\,; \qquad w_c \to 0 \quad \text{as} \quad |y| \to \infty\,. \tag{A.10 a}$$

This is a classic problem in electrostatics, and it is well-known that the far-field behavior of w_c is

$$w_c \sim \frac{C_j}{|y|} + \frac{P_j \cdot y}{|y|^3} + \cdots \qquad \text{as} \quad |y| \to \infty\,. \tag{A.10 b}$$

Here C_j is the capacitance of Ω_j and P_j denotes the dipole vector, both determined by the shape of Ω_j. These intrinsic quantities can be found explicitly for different trap shapes such as spheres, ellipsoids, etc..

Upon substituting (A.10 b) into (A.8), we obtain that the matching condition becomes

$$\frac{1}{|\Omega|^{1/2}} + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots \sim \frac{1}{|\Omega|^{1/2}}\left(1 - \frac{\varepsilon C_j}{|x - x_j|} - \frac{\varepsilon^2 P_j \cdot (x - x_j)}{|x - x_j|^3}\right) + \varepsilon w_1 + \varepsilon^2 w_2 + \cdots\,. \tag{A.11}$$

Therefore, we require that u_1 has the singular behavior $u_1 \sim -|\Omega|^{-1/2} C_j/|x - x_j|$ as $x \to x_j$ for $j = 1, \ldots, N$. The problem (A.3) for u_1 with this singularity behavior can be written in Ω in terms of the Dirac distribution as

$$\Delta u_1 = -\lambda_1 u_0 + \frac{4\pi}{|\Omega|^{1/2}} \sum_{j=1}^{N} C_j \delta(x - x_j)\,, \quad x \in \Omega\,; \qquad \partial_n u_1 = 0\,, \quad x \in \partial\Omega\,, \tag{A.12}$$

with $\int_\Omega u_1\, dx = 0$. Upon using the divergence theorem, and recalling that $u_0 = |\Omega|^{-1/2}$, we determine λ_1 as

$$\lambda_1 = \frac{4\pi}{|\Omega|} \sum_{j=1}^{N} C_j \, . \tag{A.13}$$

This leading order asymptotics is Ozawa's result [**51**], and since it does not depend on the trap locations it does not indicate how to optimize λ. As such, we must extend the calculation to one higher order.

To solve (A.12), we introduce the Neumann Green's function $G(x;\xi)$, which satisfies

$$\Delta G = \frac{1}{|\Omega|} - \delta(x-\xi)\,, \quad x \in \Omega\,; \qquad \partial_n G = 0\,, \quad x \in \partial\Omega\,, \tag{A.14 a}$$

$$G(x;\xi) = \frac{1}{4\pi|x-\xi|} + R(x;\xi)\,; \qquad \int_\Omega G(x;\xi)\, dx = 0\,. \tag{A.14 b}$$

Here $R(x;\xi)$ is called the regular part of $G(x;\xi)$, and $R(\xi;\xi)$ is referred to as the self-interaction term. In terms of G, the unique solution to (A.12), which satisfies $\int_\Omega u_1\, dx = 0$, is simply

$$u_1 = -\frac{4\pi}{|\Omega|^{1/2}} \sum_{k=1}^{N} C_k G(x;x_k)\,. \tag{A.15}$$

Next, we expand u_1 in (A.15) as $x \to x_j$. Upon using (A.14 b) to obtain the local behavior of G, we obtain

$$u_1 \sim -\frac{C_j}{|\Omega|^{1/2}|x-x_j|} + A_j \qquad \text{as} \quad x \to x_j\,; \qquad A_j = -\frac{4\pi}{|\Omega|^{1/2}} \left(C_j R_{j,j} + \sum_{\substack{k=1 \\ k\neq i}}^{N} C_k G_{j,k} \right)\,. \tag{A.16}$$

Here we have defined $R_{j,j} \equiv R(x_j;x_j)$ and $G_{j,k} \equiv G(x_j;x_k)$. Upon substituting this expression into the matching condition (A.11), we obtain

$$\frac{1}{|\Omega|^{1/2}} + \varepsilon\left(-\frac{C_j}{|\Omega|^{1/2}|x-x_j|} + A_j \right) + \varepsilon^2 u_2 + \cdots \sim \frac{1}{|\Omega|^{1/2}} \left(1 - \frac{\varepsilon C_j}{|x-x_j|} - \frac{\varepsilon^2 P_j \cdot (x-x_j)}{|x-x_j|^3} \right) + \varepsilon w_1 + \varepsilon^2 w_2 + \cdots\,. \tag{A.17}$$

We then conclude that $w_1 \sim A_j$ as $|y| \to \infty$. The solution w_1 to (A.7) is

$$w_1 = A_j\,(1-w_c) \sim A_j \left(1 - \frac{C_j}{|y|} + \cdots \right) \qquad \text{as} \quad |y| \to \infty\,, \tag{A.18}$$

where w_c is the solution to (A.10). Next, we write the far-field behavior in (A.18) in outer variables and substitute the resulting expression into the right-hand side of the matching condition (A.17) to identify the terms of $\mathcal{O}(\varepsilon^2)$. In this way, we obtain that the outer eigenfunction u_2 must have the following singularity behavior as $x \to x_j$:

$$u_2 \sim -\frac{A_j C_j}{|x-x_j|} - \frac{P_j \cdot (x-x_j)}{|x-x_j|^3} \qquad \text{as} \quad x \to x_j\,, \quad j = 1,\ldots,N\,. \tag{A.19}$$

The problem (A.4) for u_2, together with singularity behavior (A.19), can be written in Ω in terms of the Dirac distribution as

$$\Delta u_2 = -\lambda_2 u_0 - \lambda_1 u_1 + 4\pi \sum_{j=1}^{N} A_j C_j \delta(x-x_j) - 4\pi \sum_{j=1}^{N} P_j \cdot \nabla\delta(x-x_j)\,, \quad x \in \Omega\,, \tag{A.20}$$

with $\partial_n u_2 = 0$ for $x \in \partial\Omega$. Then, applying the divergence theorem to (A.20), and using $\int_\Omega u_1\, dx = 0$, we get

$$\lambda_2 = \frac{4\pi}{|\Omega|^{1/2}} \sum_{j=1}^{N} A_j C_j\,. \tag{A.21}$$

We remark that this eigenvalue correction λ_2 does not depend on the dipole vector P_j defined in (A.10 b).

Next, it is convenient to introduce the capacitance vector c and the symmetric Neumann Green's matrix $\mathcal{G}$ by (2.23). In (2.23), C_j is the capacitance defined in (A.10 b), and $G_{i,j} \equiv G(x_i; x_j)$ for $i \neq j$ is the Neumann Green's function of (A.14) with self-interaction $R_{j,j} \equiv R(x_j; x_j)$. Upon substituting (A.13) and (A.21) into (A.1), we obtain Principal Result 2.1.

Solution to Problem 2.2:

In the outer region, we expand u as

$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots \,. \tag{A.22}$$

Here u_0 is an unknown constant, and u_k for $k = 1, 2$ satisfies

$$\Delta u_k = 0\,, \quad x \in \Omega \backslash \{x_1, \ldots, x_N\}\,; \qquad \partial_n u_k = 0\,, \quad x \in \partial\Omega\,, \tag{A.23}$$

with certain singularity conditions as $x \to x_j$ for $j = 1, \ldots, N$ determined upon matching to the inner solution.

In the inner region near the j^{th} trap, we expand the inner solution $w(y) \equiv u(x_j + \varepsilon y)$, with $y \equiv \varepsilon^{-1}(x - x_j)$, as

$$w = w_0 + \varepsilon w_1 + \cdots \,. \tag{A.24}$$

Upon substituting (A.24) into (2.29 a) and (2.29 b), we obtain that w_0 and w_1 satisfy

$$\Delta_y w_0 = 0\,, \quad y \notin \Omega_j\,; \qquad w_0 = \delta_{j1}\,, \quad y \in \partial\Omega_j\,, \tag{A.25 a}$$

$$\Delta_y w_1 = 0\,, \quad y \notin \Omega_j\,; \qquad w_1 = 0\,, \quad y \in \partial\Omega_j\,. \tag{A.25 b}$$

Here $\Omega_j = \varepsilon^{-1}\Omega_{\varepsilon_j}$, and δ_{j1} is Kronecker's symbol. The far-field boundary conditions for w_0 and w_1 are determined by the matching condition as $x \to x_j$ between the the inner and outer expansions (A.24) and (A.22), respectively, written as

$$u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots \sim w_0 + \varepsilon w_1 + \cdots \,. \tag{A.26}$$

The first matching condition is that $w_0 \sim u_0$ as $|y| \to \infty$, where u_0 is an unknown constant. Then, the solution for w_0 in the j^{th} inner region is given by

$$w_0 = u_0 + (\delta_{j1} - u_0)\, w_c(y)\,, \tag{A.27}$$

where w_c is the solution to (A.10 a). Upon, using the far-field asymptotic behavior (A.10 b) for w_c, we obtain that

$$w_0 \sim u_0 + (\delta_{j1} - u_0) \left(\frac{C_j}{|y|} + \frac{P_j \cdot y}{|y|^3} \right)\,, \quad \text{as } \; y \to \infty\,. \tag{A.28}$$

Here C_j and P_j are the capacitance and dipole vector of Ω_j, respectively, as defined in (A.10 b).

From (A.28) and (A.26), we conclude that u_1 satisfies (A.23) with singular behavior $u_1 \sim (\delta_{j1} - u_0)\, C_j/|x - x_j|$ as $x \to x_j$ for $j = 1, \ldots, N$. Therefore, in terms of the Dirac distribution, u_1 satisfies

$$\Delta u_1 = -4\pi \sum_{j=1}^{N} (\delta_{j1} - u_0)\, C_j \delta(x - x_j)\,, \quad x \in \Omega\,; \qquad \partial_n u_1 = 0\,, \quad x \in \partial\Omega\,. \tag{A.29}$$

The solvability condition for u_1, obtained by the divergence theorem, determines the unknown constant u_0 as

$$u_0 = \frac{C_1}{N\bar{C}}\,, \qquad \bar{C} \equiv \frac{1}{N}\left(C_1 + \cdots C_N\right)\,. \tag{A.30}$$

In terms of the Neumann Green's function of (A.14), and an unknown constant χ_1, the solution to (A.29) is

$$u_1 = 4\pi \sum_{i=1}^{N} \left(\delta_{i1} - u_0\right) C_i G(x;x_i) + \chi_1\,, \qquad \chi_1 = \frac{1}{|\Omega|}\int_\Omega u_1\,dx\,. \tag{A.31}$$

Next, by expanding u_1 as $x \to x_j$, and using the local behavior $G(x;x_i) \sim 1/(4\pi|x-x_i|) + R_{i,i}$ of G as $x \to x_i$ from (A.14 b), we obtain that

$$u_1 \sim \begin{cases} \frac{(1-u_0)C_1}{|x-x_1|} + A_1 + \chi_1\,, & \text{as } x \to x_1\,, \\ -\frac{-u_0 C_j}{|x-x_j|} + A_j + \chi_1\,, & \text{as } x \to x_j\,, \ \ j = 2,\ldots,N\,. \end{cases} \tag{A.32 a}$$

Here, the constants A_j for $j = 1,\ldots,N$ are defined by

$$A_1 = 4\pi C_1 R_{1,1} - 4\pi u_0 \left(C_1 R_{1.1} + \sum_{i=2}^{N} C_i G_{1,i} \right)\,; \quad A_j = 4\pi C_1 G_{j,1} - 4\pi u_0 \left(C_j R_{j,j} + \sum_{\substack{j=1 \\ j\neq i}}^{N} C_i G_{j,i} \right)\,, \quad j = 2,\ldots,N\,. \tag{A.32 b}$$

Upon substituting (A.32) into the matching condition (A.26), we obtain that the solution w_1 to (A.25 b) must satisfy $w_1 \sim A_j + \chi_1$ as $|y| \to \infty$. Thus, $w_1 = (A_j + \chi_1)(1 - w_c)$, where w_c is the solution to (A.10 a). Upon, using the far-field behavior (A.10 b) for w_c, and substituting the resulting expression into the matching condition (A.26), we obtain that u_2 satisfies (A.23) with singularity behavior

$$u_2 \sim -\frac{C_j\left(A_j + \chi_1\right)}{|x-x_j|} + \left(\delta_{j1} - u_0\right)\frac{P_j \cdot (x - x_j)}{|x-x_j|^3}\,, \quad \text{as } x \to x_j\,, \quad j = 1,\ldots,N\,. \tag{A.33}$$

Therefore, in terms of distributions, u_2 satisfies

$$\Delta u_2 = 4\pi \sum_{j=1}^{N} C_j\left(A_j + \chi_1\right)\delta(x - x_j) + 4\pi \sum_{j=1}^{N} \left(\delta_{j1} - u_0\right) P_j \cdot \nabla\delta(x - x_j)\,, \quad x \in \Omega\,, \tag{A.34}$$

with $\partial_n u_2 = 0$ on $x \in \partial\Omega$. The solvability condition for u_2, obtained by the divergence theorem, determines χ_1 as

$$\chi_1 = -\frac{1}{N\bar{C}} \sum_{j=1}^{N} A_j C_j\,. \tag{A.35}$$

Finally, we substitute (A.32 b) for A_j into (A.35) and write the resulting expression for χ_1 in matrix form by using the Green's matrix $\mathcal{G}$ of (2.23). In this way, we obtain Principal Result 2.3.

Appendix B Solutions to the Problems in §3

Solution to Problem 3.1:

In the outer region, defined away from Ω_{ε_j} for $j = 1,\ldots,N$, we expand

$$u(x;\varepsilon) \sim U_{0H}(x) + U_0(x;\boldsymbol{\nu}) + \sigma(\varepsilon)U_1(x;\boldsymbol{\nu}) + \cdots\,. \tag{B.1}$$

Here $\boldsymbol{\nu} = (\nu_1,\ldots,\nu_N)$ is a set of logarithmic gauge functions to be determined and $\sigma \ll \nu_j^k$ as $\varepsilon \to 0$ for $j = 1,\ldots,N$.

In (B.1), $U_{0H}(x)$ is the smooth function satisfying the unperturbed problem in the unperturbed domain Ω

$$\triangle U_{0H} - m(x) U_{0H} = 0\,, \quad x \in \Omega\,; \qquad U_{0H} = f\,, \quad x \in \partial\Omega\,. \tag{B.2}$$

Substituting (B.1) into (3.39 a) and (3.39 c), and letting $\Omega_{\varepsilon_j} \to x_j$ as $\varepsilon \to 0$, we get that U_0 satisfies

$$\triangle U_0 - m(x) U_0 = 0\,, \quad x \in \Omega \backslash \{x_1, \ldots, x_N\}\,, \tag{B.3 a}$$

$$U_0 = 0\,, \qquad x \in \partial\Omega\,, \tag{B.3 b}$$

$$U_0 \quad \text{is singular as} \quad x \to x_j\,, \quad j = 1, \ldots, N\,. \tag{B.3 c}$$

The singularity behavior for U_0 as $x \to x_j$ will be found below by matching the outer solution to the far-field behavior of the inner solution to be constructed near each Ω_{ε_j}.

In the j^{th} inner region near Ω_{ε_j} we introduce the inner variables y and $v(y;\varepsilon)$ by

$$y = \varepsilon^{-1}(x - x_j)\,, \qquad v(y;\varepsilon) = u(x_j + \varepsilon y; \varepsilon)\,. \tag{B.4}$$

We then expand $v(y;\varepsilon)$ as

$$v(y;\varepsilon) = \alpha_j + \nu_j \gamma_j v_{cj}(y) + \mu_0(\varepsilon) V_{1j}(y) + \cdots\,, \tag{B.5}$$

where $\gamma_j = \gamma_j(\boldsymbol{\nu})$ is a constant to be determined. Here $\mu_0 \ll \nu_j^k$ as $\varepsilon \to 0$ for any $k > 0$. In (B.5), the logarithmic gauge function ν_j is defined by

$$\nu_j = -1/\log(\varepsilon d_j)\,, \tag{B.6}$$

where d_j is specified below. By substituting (B.4) and (B.5) into (3.39 a) and (3.39 b), we conclude that $v_{cj}(y)$ is the unique solution to

$$\triangle_y v_{cj} = 0\,, \quad y \notin \Omega_j\,; \quad v_{cj} = 0\,, \quad y \in \partial\Omega_j\,, \tag{B.7 a}$$

$$v_{cj}(y) \sim \log|y| - \log d_j + o(1)\,, \quad \text{as} \quad |y| \to \infty\,. \tag{B.7 b}$$

Here $\Omega_j \equiv \varepsilon^{-1}\Omega_{\varepsilon_j}$, and the logarithmic capacitance, d_j, is determined by the shape of Ω_j.

Writing (B.7 b) in outer variables and substituting the result into (B.5), we get that the far-field expansion of v away from each Ω_j is

$$v \sim \alpha_j + \gamma_j + \nu_j \gamma_j \log|x - x_j|\,, \qquad j = 1, \ldots, N\,. \tag{B.8}$$

Then, by expanding the outer solution (B.1) as $x \to x_j$, we obtain the following matching condition between the inner and outer solutions:

$$U_{0H}(x_j) + U_0 \sim \alpha_j + \gamma_j + \nu_j \gamma_j \log|x - x_j|\,, \quad \text{as} \quad x \to x_j\,, \quad j = 1, \ldots, N\,. \tag{B.9}$$

In this way, we obtain that U_0 satisfies (B.3) subject to the singularity structure

$$U_0 \sim \alpha_j - U_{0H}(x_j) + \gamma_j + \nu_j \gamma_j \log|x - x_j| + o(1)\,, \quad \text{as} \quad x \to x_j\,, \quad j = 1, \ldots, N\,. \tag{B.10}$$

Observe that in (B.10) both the singular and regular parts of the singularity structure are specified. Therefore, (B.10) will effectively lead to a linear system of algebraic equations for γ_j for $j = 1, \ldots, N$.

The solution to (B.3 *a*) and (B.3 *b*), with $U_0 \sim \nu_j \gamma_j \log|x - x_j|$ as $x \to x_j$, can be written as

$$U_0(x; \boldsymbol{\nu}) = -2\pi \sum_{i=1}^{N} \nu_i \gamma_i G(x; x_i) \,, \tag{B.11}$$

where $G(x; x_j)$ is the Green's function satisfying

$$\triangle G - m(x) G = -\delta(x - x_j) \,, \quad x \in \Omega \,; \quad G = 0 \,, \quad x \in \partial\Omega \,, \tag{B.12 a}$$

$$G(x; x_j) \sim -\frac{1}{2\pi} \log|x - x_j| + R(x_j; x_j) + o(1) \,, \quad \text{as} \quad x \to x_j \,. \tag{B.12 b}$$

Here $R_{jj} \equiv R(x_j; x_j)$ is the regular part of G.

Finally, we expand (B.11) as $x \to x_j$ and equate the resulting expression with the required singularity behavior (B.10) to get

$$\nu_j \gamma_j \log|x - x_j| - 2\pi \nu_j \gamma_j R_{jj} - 2\pi \sum_{\substack{i=1 \\ i \neq j}}^{N} \nu_i \gamma_i G(x_j; x_i) = \alpha_j - U_{0H}(x_j) + \gamma_j + \nu_j \gamma_j \log|x - x_j| \,, \quad j = 1, \ldots, N \,. \tag{B.13}$$

In this way, we get the following linear algebraic system for γ_j for $j = 1, \ldots, N$:

$$-\gamma_j \left(1 + 2\pi \nu_j R_{jj}\right) - 2\pi \sum_{\substack{i=1 \\ i \neq j}}^{N} \nu_i \gamma_i G_{ji} = \alpha_j - U_{0H}(x_j) \,, \quad j = 1, \ldots, N \,. \tag{B.14}$$

Here $G_{ji} \equiv G(x_j; x_i)$ and $\nu_j = -1/\log(\varepsilon d_j)$. We summarize the asymptotic construction as follows:

Principal Result: For $\varepsilon \ll 1$, the outer expansion for (3.39) is

$$u \sim U_{0H}(x) - 2\pi \sum_{i=1}^{N} \nu_i \gamma_i G(x; x_i) \,, \quad \text{for} \quad |x - x_j| = \mathcal{O}(1) \,. \tag{B.15 a}$$

The inner expansion near Ω_{ε_j} with $y = \varepsilon^{-1}(x - x_j)$, is

$$u \sim \alpha_j + \nu_j \gamma_j v_{cj}(y) \,, \quad \text{for} \quad |x - x_j| = \mathcal{O}(\varepsilon) \,. \tag{B.15 b}$$

Here $\nu_j = -1/\log(\varepsilon d_j)$, d_j is defined in (B.7 *b*), $v_{cj}(y)$ satisfies (B.7), U_{0H} satisfies the unperturbed problem (B.2), while $G(x; x_j)$ and $R(x_j; x_j)$ satisfy (B.12). Finally, the constants γ_j for $j = 1, \ldots, N$ are obtained from the N dimensional linear algebraic system (B.14).

To illustrate the theory, let Ω be the unit disk containing one arbitrarily-shaped hole centered at the origin. Suppose that $m(x) = 1$ and $f = 0$. Then, $U_{0H} \equiv 0$, and the Green's function satisfying (B.12) is radially symmetric with a singularity at the center of the disk. The explicit Green's function is

$$G(x; \mathbf{0}) = \frac{1}{2\pi} \left[K_0(r) - \frac{K_0(1)}{I_0(1)} I_0(r) \right] \,, \quad 0 < r < 1 \,, \tag{B.16}$$

where $r \equiv |x|$. Here $I_0(r)$ and $K_0(r)$ are the modified Bessel functions of the first and second kind, respectively, of order zero. To identity the regular part of G at the origin, i.e. $R(\mathbf{0}; \mathbf{0})$, we use the well-known asymptotics $K_0(r) \sim -\log r + \log 2 - \gamma_e$ as $r \to 0$, where γ_e is Euler's constant. Then, from (B.16) and (B.12 *b*), we get that

$$R_{11} \equiv R(\mathbf{0}; \mathbf{0}) = \frac{1}{2\pi} \left[\log 2 - \gamma_e - \frac{K_0(1)}{I_0(1)} \right] \,. \tag{B.17}$$

For $N = 1$, $U_{0H} \equiv 0$, and $\alpha_1 = 1$, the system (B.14) then determines γ_1 in terms of R_{11} and $\nu = -1/\log(\varepsilon d_1)$ as

$$\gamma_1 = -\left[1 + 2\pi\nu_1 R_{11}\right]^{-1} . \tag{B.18}$$

Therefore, γ_1 is determined explicitly in terms of the logarithmic capacitance, d_1, of the arbitrarily-shaped hole centered at the origin.

Solution to Problem 3.2:

This is just a simple application of the theory in Problem 2 for the special case of a disk of radius 2 with $m(x) \equiv 0$ and $f = 4\cos(2\theta) = 4(\cos^2\theta - \sin^2\theta) = x^2 - y^2$ on $(x^2 + y^2)^{1/2} = 4$.

For this problem, the solution to the unperturbed problem (B.2) is simply

$$U_{0H}(x, y) = x^2 - y^2 . \tag{B.19}$$

Next, the Green's function satisfying (B.12) of Problem 2 with $m(x) \equiv 0$ and its regular part are calculated from the method of images as

$$G(x; x_j) = -\frac{1}{2\pi} \log\left(\frac{2|x - x_j|}{|x - x_j{}'||x_j|}\right) , \qquad R_{jj} \equiv R(x_j; x_j) = -\frac{1}{2\pi} \log\left[\frac{2}{|x_j - x_j{}'||x_j|}\right] . \tag{B.20}$$

Here $x_j{}'$ is the image point of x_j in the unit disk of radius two..

Next, we note that since each of the holes has an elliptic shape with semi-axes ε and 2ε, then from Table 1 of the notes their common logarithmic capacitance is $d = 3/2$. The holes are assumed to be centered at $x_1 = (1/2, 1/2)$, $x_2 = (1/2, 0)$ and $x_3 = (-1/4, 0)$, and have the constant boundary values $\alpha_1 = 1$, $\alpha_2 = 0$ and $\alpha_3 = 2$.

Therefore, upon defining $\nu = -1/\log(3\varepsilon/2)$ we obtain from (B.14) of Problem 2 that γ_j for $j = 1, \ldots, 3$ is the solution of the linear system

$$-\gamma_1\left[1 + 2\pi\nu R_{11}\right] - 2\pi\nu\left[\gamma_2 G(x_1; x_2) + \gamma_3 G(x_1; x_3)\right] = 1 , \tag{B.21 a}$$

$$-\gamma_2\left[1 + 2\pi\nu R_{22}\right] - 2\pi\nu\left[\gamma_1 G(x_2; x_1) + \gamma_3 G(x_2; x_3)\right] = -1/4 , \tag{B.21 b}$$

$$-\gamma_3\left[1 + 2\pi\nu R_{33}\right] - 2\pi\nu\left[\gamma_1 G(x_3; x_1) + \gamma_2 G(x_3; x_2)\right] = 31/16 . \tag{B.21 c}$$

Here R_{jj} and $G(x_j; x_i)$ are to be evaluated from (B.20).

We solve this linear system numerically for γ_j as a function of ε. The curves $\gamma_j(\varepsilon)$ as a function of ε are plotted in Fig. B 1. We observe that the leading-order approximation to (B.21), valid for $\nu \ll 1$, is simply $\gamma_1 = -1$, $\gamma_2 = 1/4$ and $\gamma_3 = -31/16$. From Fig. B 1 we observe that this approximation, which neglects interaction effects between the holes, is rather inaccurate unless ε is very small.

Solution to Problem 3.3:

The analysis in §5.3 of the notes can be repeated, and we readily obtain that the infinite-order logarithmic series approximation $\lambda^\star$ to the principal eigenvalue λ satisfies the transcendental equation

$$R_h(x_0; x_0, \lambda^*) = -\frac{1}{2\pi\nu} , \qquad \nu = -\frac{1}{\log(\varepsilon d)} , \tag{B.22}$$

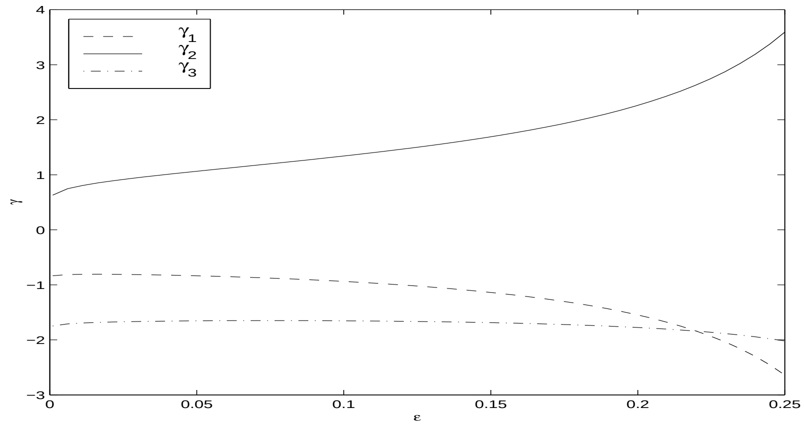


FIGURE B 1. Plot of $\gamma_j = \gamma_j(\epsilon)$ for $j = 1, 2, 3$ obtained from the numerical solution to (B.21).

where $R_h(x_0; x_0, \lambda^*)$ is the regular part of the Helmholtz Green's function, satisfying

$$\Delta G_h + \lambda^* G_h = -\delta(x - x_0)\,, \quad x \in \Omega\,; \quad G_h = 0\,, \quad x \in \partial\Omega\,, \tag{B.23 a}$$

$$G_h(x; x_0, \lambda^*) \sim -\frac{1}{2\pi} \log|x - x_0| + R_h(x_0; x_0, \lambda^*) + o(1)\,, \quad \text{as} \quad x \to x_0\,. \tag{B.23 b}$$

Notice that $G_h = 0$ on $\partial\Omega$. Since the hole is centered at the origin then $x_0 = 0$.

When Ω is the unit disk with a hole centered at the origin, then (B.23) becomes a radially symmetric problem whose solution can be found explicitly. A simple calculation gives

$$G = -\frac{1}{4}\left[Y_0\left(\sqrt{\lambda^\star} r\right) - \frac{Y_0\left(\sqrt{\lambda^\star}\right)}{J_0\left(\sqrt{\lambda^\star}\right)} J_0\left(\sqrt{\lambda^\star} r\right) \right]\,, \quad 0 < r < 1\,, \tag{B.24}$$

where $r = |x|$. Here $J_0(z)$ and $Y_0(z)$ are the Bessel functions of the first and second kind, of order zero. By using the well-known asymptotic behavior $Y_0(z) \sim 2\pi^{-1}\left[\log z - \log 2 + \gamma_e + o(1)\right]$ and $J_0(z) \sim 1 + o(1)$ as $z \to 0^+$, we obtain from (B.24) that the local behavior for G as $x \to 0$ is given by

$$G(x; \mathbf{0}) \sim -\frac{1}{2\pi} \log|x| + R_h + o(1)\,, \quad \text{as} \quad x \to \mathbf{0}\,, \tag{B.25 a}$$

$$R_h \equiv -\frac{1}{2\pi}\left(-\log 2 + \gamma_e + \log\left(\sqrt{\lambda^\star}\right)\right) + \frac{1}{4}\left(\frac{Y_0\left(\sqrt{\lambda^\star}\right)}{J_0\left(\sqrt{\lambda^\star}\right)} \right)\,, \tag{B.25 b}$$

where γ_e is Euler's constant. Finally, upon substituting (B.25 b) for R_h into (B.22), we conclude that $\lambda^\star(\varepsilon d)$ is the first root of the transcendental equation

$$\log 2 - \gamma_e - \log\left(\sqrt{\lambda^\star}\right) + \frac{\pi}{2}\left(\frac{Y_0\left(\sqrt{\lambda^\star}\right)}{J_0\left(\sqrt{\lambda^\star}\right)} \right) = -\frac{1}{\nu} = \log(\varepsilon d)\,. \tag{B.26}$$

Here d is the logarithmic capacitance of the arbitrarily-shaped hole centered at the origin of the unit disk.

It is interesting to note that the result (B.26) can also be obtained by first finding the exact eigenvalue relation for the concentric annulus $\varepsilon < |x| < 1$ with $u = 0$ on $|x| = \varepsilon$ and on $|x| = 1$, and then letting $\varepsilon \to 0$ in this resulting expression. The eigenfunction is proportional to

$$u = \left[J_0\left(\sqrt{\lambda} r\right) - \frac{J_0\left(\sqrt{\lambda}\right)}{Y_0\left(\sqrt{\lambda}\right)} Y_0\left(\sqrt{\lambda} r\right) \right], \quad 0 < r < 1, \tag{B.27}$$

and upon setting $u = 0$ at $r = \varepsilon$, we get the eigenvalue relation

$$Y_0\left(\sqrt{\lambda}\varepsilon\right) = J_0\left(\sqrt{\lambda}\varepsilon\right) \frac{Y_0\left(\sqrt{\lambda}\right)}{J_0\left(\sqrt{\lambda}\right)}. \tag{B.28}$$

Next, in (B.28) we use the small argument expansions of $Y_0(z)$ and $J_0(z)$ as $z \to 0^+$, and then, finally, replace ε by εd in the resulting expression by recalling Kaplun's equivalence principle. In this way, we readily recover the transcendental equation (B.26) for the approximation $\lambda^\star$ to λ.

Solution to Problem 3.4:

We write the eigenvalue problem as

$$\triangle u + \lambda u = 0, \quad x \in \Omega \backslash \Omega_p; \qquad \Omega_p \equiv \cup_{j=1}^{K} \Omega_{\varepsilon_j}, \tag{B.29 a}$$

$$\partial_n u = 0, \quad x \in \partial\Omega; \qquad \int_{\Omega\backslash\Omega_p} u^2\, dx = 1 \tag{B.29 b}$$

$$u = 0, \quad x \in \partial\Omega_{\varepsilon_j}, \quad j = 1, \ldots, N. \tag{B.29 c}$$

We assume that each hole Ω_{ε_j} is centered at $x_j \in \Omega$ and has the same logarithmic capacitance d.

We look for a two-term expansion for the principal eigenvalue $\lambda_0(\varepsilon)$ as

$$\lambda_0(\varepsilon) = \lambda_1 \nu + \lambda_2 \nu^2 + \cdots, \qquad \nu = -1/\log(\varepsilon d). \tag{B.30}$$

In the outer region, away from $\mathcal{O}(\varepsilon)$ neighborhoods of the holes, we expand the outer solution for u as

$$u = u_0 + \nu u_1 + \nu^2 u_2 + \cdots. \tag{B.31}$$

The leading-order term is

$$u_0 = |\Omega|^{-1/2}, \tag{B.32}$$

where $|\Omega|$ is the area of Ω. Upon substituting (B.30) and (B.31) into (B.29 a) and (B.29 b), and collecting powers of ν, we obtain that u_1 satisfies

$$\triangle u_1 = -\lambda_1 u_0, \quad x \in \Omega \backslash \{x_1, \ldots, x_K\}; \qquad \int_\Omega u_1\, dx = 0, \tag{B.33 a}$$

$$\partial_n u_1 = 0, \quad x \in \partial\Omega; \quad u_1 \text{ singular as } x \to x_j, \quad j = 1, \ldots, K, \tag{B.33 b}$$

while u_2 satisfies

$$\triangle u_2 = -\lambda_2 u_0 - \lambda_1 u_1, \quad x \in \Omega \backslash \{x_1, \ldots, x_K\}; \qquad \int_\Omega \left(u_1^2 + 2u_0 u_2\right)\, dx = 0, \tag{B.34 a}$$

$$\partial_n u_2 = 0, \quad x \in \partial\Omega; \quad u_2 \text{ singular as } x \to x_j, \quad j = 1, \ldots, K. \tag{B.34 b}$$

Now in the j^{th} inner region we introduce the new variables by

$$y = \varepsilon^{-1}(x - x_j)\,, \qquad v(y) = u(x_j + \varepsilon y)\,. \tag{B.35}$$

We then expand the inner solution as

$$v(y) = \nu A_{0j} v_{cj}(y) + \nu^2 A_{1j} v_{cj}(y) + \cdots\,. \tag{B.36}$$

Upon substituting (B.35) and (B.36) into (B.29 a) and (B.29 c), we obtain that v_{cj} satisfies

$$\triangle_y v_{cj} = 0\,, \quad y \notin \Omega_j\,; \quad v_{cj} = 0\,, \quad y \in \partial\Omega_j\,, \tag{B.37 a}$$

$$v_{cj}(y) \sim \log|y| - \log d + o(1)\,, \quad \text{as} \quad |y| \to \infty\,. \tag{B.37 b}$$

Here $\triangle_y$ is the Laplacian in the y variable, and $\Omega_j \equiv \varepsilon^{-1}\Omega_{\varepsilon_j}$. We consider the special case where d is independent of j.

Upon using the far-field form (B.37 b) in (B.36), and writing the resulting expression in outer variables, we get

$$v = A_{0j} + \nu\left[A_{0j}\log|x - x_j| + A_{1j}\right] + \nu^2\left[A_{1j}\log|x - x_j| + A_{2j}\right] + \cdots\,. \tag{B.38}$$

The far-field behavior (B.38) must agree with the local behavior of the outer expansion (B.31). Therefore, we obtain that

$$A_{0j} = u_0 = |\Omega|^{-1/2}\,, \quad j = 1, \ldots K\,, \tag{B.39 a}$$

$$u_1 \sim u_0 \log|x - x_j| + A_{1j}\,, \quad \text{as} \quad x \to x_j\,, \quad j = 1, \ldots, K\,, \tag{B.39 b}$$

$$u_2 \sim A_{1j}\log|x - x_j| + A_{2j}\,, \quad \text{as} \quad x \to x_j\,, \quad j = 1, \ldots, K\,. \tag{B.39 c}$$

Equations (B.39 b) and (B.39 c) give the required singularity structure for u_1 and u_2 in (B.33) and (B.34), respectively.

The problem for u_1 with singular behavior (B.39 b) can be written in terms of the delta function as

$$\triangle u_1 = -\lambda_1 u_0 + 2\pi A_0 \sum_{j=1}^{K} \delta(x - x_j)\,, \quad x \in \Omega\,; \qquad \int_\Omega u_1\, dx = 0\,, \tag{B.40 a}$$

$$\partial_n u_1 = 0\,, \quad x \in \partial\Omega\,. \tag{B.40 b}$$

Upon using the divergence theorem we obtain that $-\lambda_1 u_0 \int_\Omega 1 dx + 2\pi A_0 K = 0$, so that with $u_0 = A_0$ from (B.39 a), we get

$$\lambda_1 = \frac{2\pi K}{|\Omega|}\,. \tag{B.41}$$

The solution to (B.40) can be written in terms of the Neumann Green's function as

$$u_1 = -2\pi u_0 \sum_{i=1}^{K} G_N(x; x_i)\,, \tag{B.42}$$

where the Neumann Green's function $G_N(x;\xi)$ satisfies (3.55). Since G_N has a zero spatial average, it follows from (B.42) that $\int_\Omega u_1\, dx = 0$, as required in (B.40 a).

Next, we expand u_1 as $x \to x_j$. We use the local behavior for G_N, given in (3.55 d), to obtain from (B.42) that

$$u_1 \sim u_0 \log |x - x_j| - 2\pi u_0 \left[R_{Njj} + \sum_{\substack{i=1 \\ i \neq j}}^{K} G_{Nij} \right] , \quad x \to x_j \, , \tag{B.43}$$

where $G_{Nji} = G_N(x_j; x_i)$ and $R_{Njj} = R_N(x_j; x_j)$. Comparing (B.43) and the required singularity behavior (B.39 b), we obtain that

$$A_{1j} = -2\pi u_0 \left[R_{Njj} + \sum_{\substack{i=1 \\ i \neq j}}^{K} G_{Nij} \right] , \qquad j = 1, \ldots, N \, . \tag{B.44}$$

Next, we write the problem (B.34) in Ω as

$$\triangle u_2 = -\lambda_2 u_0 - \lambda_1 u_1 + 2\pi \sum_{j=1}^{K} A_{1j} \delta(x - x_j) \, , \quad x \in \Omega \, ; \quad \partial_n u_2 = 0 \, , \quad x \in \partial\Omega \, . \tag{B.45}$$

Since $\int_\Omega u_1 \, dx = 0$ and $u_0 = |\Omega|^{-1/2}$, the divergence theorem applied to (B.45) determines λ_2 as $\lambda_2 u_0 |\Omega| = 2\pi \sum_{j=1} A_{1j}$. Finally, we use (B.44) for A_{1j}, we get

$$\lambda_2 = -\frac{4\pi^2}{|\Omega|} p(x_1, \ldots, x_K) \, , \qquad p(x_1, \ldots, x_K) \equiv \sum_{j=1}^{N} \left(R_{Njj} + \sum_{\substack{i=1 \\ i \neq j}}^{K} G_{Nji} \right) \, . \tag{B.46}$$

Combining (B.30) with (B.41) and (B.46) we get the two-term expansion given in equations (5.27) and (5.28) of the Corollary in §5 of the workshop notes given by

$$\lambda_0(\varepsilon) \sim \frac{2\pi\nu K}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|} p(x_1, \ldots, x_K) + \cdots \, , \qquad \nu = -1/\log(\varepsilon d) \, . \tag{B.47}$$

Appendix C Solutions to the Problems in §4

Solution to Problem 4.1:

We now derive the leading-order term in the asymptotic expansion for the positive principal eigenvalue of (4.49), as given in Principal Result 4.3. We expand λ as in (4.8), and we expand the outer representation for the eigenfunction ϕ as in (4.9). Upon substituting (4.8) and (4.9) into (4.49), we obtain that $\phi_0 = |\Omega|^{-1/2}$ is a constant, and that ϕ_1 satisfies

$$\Delta \phi_1 = \mu_0 m_b \phi_0 \, , \quad x \in \Omega \backslash \Omega^I \, ; \qquad \partial_n \phi_1 = 0 \, , \quad x \in \partial\Omega \backslash \Omega^B \, ; \qquad \int_\Omega \phi_1 \, dx = 0 \, . \tag{C.1}$$

In (C.1), we recall that $\Omega^I \equiv \{x_1, \ldots, x_n\} \cap \Omega$ denotes the set of the centers of the interior patches, while $\Omega^B \equiv \{x_1, \ldots, x_n\} \cap \partial\Omega$ denotes the set of the centers of the boundary patches.

In the inner region, near the j^{th} patch we introduce the local variables $y = \varepsilon^{-1}(x - x_j)$ and $\psi(y) = \phi(x_j + \varepsilon y)$. We then expand ψ for $y = \mathcal{O}(1)$ by

$$\psi \sim \psi_{0j} + \nu \psi_{1j} + \nu^2 \psi_{2j} + \cdots \, , \tag{C.2}$$

where ψ_{0j} is a constant to be determined. For an interior patch with $x_j \in \Omega^I$, we obtain that ψ_{1j} satisfies satisfy

$$\Delta\psi_{1j} = \begin{cases} \mathcal{F}_{1j}\,, & |y| \le \rho_j\,, \\ 0\,, & |y| \ge \rho_j\,, \end{cases} \tag{C.3}$$

where $\mathcal{F}_{1j} = -\mu_0 m_j \psi_{0j}$. The solution for ψ_{1j}, with $\rho = |y|$, is

$$\psi_{1j} = \begin{cases} A_{1j}\left(\frac{\rho^2}{2\rho_j^2}\right) + \bar{\psi}_{1j}\,, & 0 \le \rho \le \rho_j\,, \\ A_{1j}\log\left(\frac{\rho}{\rho_j}\right) + \frac{A_{1j}}{2} + \bar{\psi}_{1j}\,, & \rho \ge \rho_j\,, \end{cases} \tag{C.4}$$

where $\bar{\psi}_{1j}$ is an unknown constant. The divergence theorem is used to calculate A_{1j} from (C.3), and we get

$$A_{1j} = -\frac{\mu_0}{2} m_j \rho_j^2 \psi_{0j}\,, \qquad . \tag{C.5}$$

For a boundary patch, for which $x_j \in \Omega^B$, then (C.3) holds in the wedge $\beta_j < \arg(y) < \beta_j + \pi\alpha_j$, for some β_j and $0 < \alpha_j < 2$. For this boundary case, the constants A_{1j} are also given by (C.5).

The matching condition between the outer solution as $x \to x_j$ and the inner solution as $|y| = \varepsilon^{-1}|x - x_j| \to \infty$ is

$$\phi_0 + \nu\phi_1 + \cdots \sim \psi_{0j} + A_{1j} + \nu\left(A_{1j}\log|x - x_j| - A_{1j}\log\rho_j + \frac{A_{1j}}{2} + \bar{\psi}_{1j} + A_{2j}\right) + \nu^2\left(A_{2j}\log|x - x_j| + \mathcal{O}(1)\right)\,. \tag{C.6}$$

The leading-order matching condition from (C.6) yields

$$\phi_0 = \psi_{0j} + A_{1j}\,, \qquad j = 1, \ldots, n\,. \tag{C.7}$$

From the $\mathcal{O}(\nu)$ terms in (C.6), we obtain that ϕ_1 has the following singular behavior as $x \to x_j$

$$\phi_1 \sim A_{1j}\log|x - x_j| - A_{1j}\log\rho_j + \frac{A_{1j}}{2} + \bar{\psi}_{1j} + A_{2j}\,, \quad \text{as} \quad x \to x_j\,. \tag{C.8}$$

Next, by using the divergence theorem on the solution ϕ_1 to (C.1) with singular behavior (C.8) we obtain

$$\mu_0 m_b |\Omega| \phi_0 = -\pi \sum_{j=1}^{n} \alpha_j A_{1j}\,. \tag{C.9}$$

By combining (C.7) and (C.5) for A_{1j}, we obtain that

$$\psi_{0j} = \frac{2\phi_0}{2 - m_j\rho_j^2\mu_0}\,, \qquad A_{1j} = -\frac{m_j\rho_j^2\mu_0\phi_0}{2 - m_j\rho_j^2\mu_0}\,, \qquad j = 1, \ldots, n\,. \tag{C.10}$$

From (C.9), together with (C.10) for A_{1j}, we obtain that the leading-order eigenvalue correction μ_0 is a root of the nonlinear algebraic equation

$$\frac{m_b|\Omega|}{\pi} = \sum_{j=1}^{n} \frac{\alpha_j m_j \rho_j^2}{2 - m_j\rho_j^2\mu_0}\,. \tag{C.11}$$

This yields a transcendental equation for the leading-order term μ_0 in the expansion of the eigenvalue, as given in Principal Result 4.3.

The calculation of the higher-order term of order $\mathcal{O}(\nu^2)$, as written in Principal Result 4.3, is more involved and is given in §3 of [**45**].

Solution to Problem 4.2:

To prove Qualitative Result III, we first impose the constraint (4.62), and then calculate from (4.53) that

$$\mathcal{B}_{\text{new}}(\zeta) - \mathcal{B}_{\text{old}}(\zeta) = \frac{2\pi m_j \rho_j^2}{(2-\zeta m_j \rho_j^2)} + \frac{\pi \alpha_k m_k \rho_k^2}{(2-\zeta m_k \rho_k^2)} - \frac{2\pi m_i \rho_i^2}{(2-\zeta m_i \rho_i^2)}\,,$$

$$= \frac{\pi \alpha_k \zeta \beta_k}{(2-\zeta\beta_i)(2-\zeta\beta_j)(2-\zeta\beta_k)} \left[-4\beta_j + (2-\alpha_k)\beta_k + \zeta\beta_j \left(\beta_j + \frac{\alpha_k}{2}\beta_k \right) \right]\,, \tag{C.12 a}$$

$$= \frac{\pi \alpha_k \zeta \beta_k}{(2-\zeta\beta_i)(2-\zeta\beta_j)(2-\zeta\beta_k)} \left[-\beta_j(2-\zeta\beta_j) + 2(\beta_k - \beta_j) - \frac{\alpha_k \beta_k}{2}(2-\zeta\beta_j) \right]\,, \tag{C.12 b}$$

where we have defined $\beta_i \equiv m_i \rho_i^2$, $\beta_j \equiv m_j \rho_j^2$, and $\beta_k \equiv m_k \rho_k^2$. There are three parameter ranges of interest, corresponding to the three statements in Qualitative Result III.

We first suppose that $\beta_i > 0$ and $\beta_k > \frac{4}{2-\alpha_k}\beta_j > 0$. Then, from (4.62), it follows that $\beta_i > \beta_j$, and

$$\beta_i < \frac{(2-\alpha_k)}{4}\beta_k + \frac{\alpha_k}{2}\beta_k = \beta_k - \frac{1}{2}\left(1 - \frac{\alpha_k}{2}\right)\beta_k\,,$$

so that $\beta_i < \beta_k$ since $0 < \alpha_k < 2$. It then readily follows that the first vertical asymptote $\mu_{\text{m}}^{\text{new}}$ and $\mu_{\text{m}}^{\text{old}}$ for $\mathcal{B}_{\text{new}}(\zeta)$ and $\mathcal{B}_{\text{old}}(\zeta)$, respectively, must satisfy $\mu_{\text{m}}^{\text{new}} \le \mu_{\text{m}}^{\text{old}}$. Furthermore, it follows from (C.12 *a*) that $\mathcal{B}_{\text{new}}(\zeta) > \mathcal{B}_{\text{old}}(\zeta)$ on $0 < \zeta < \mu_{\text{m}}^{\text{new}}$. Consequently, Case I of the Lemma ensures that $\mu_0^{\text{new}} < \mu_0^{\text{old}}$. This establishes the first statement of Qualitative Result III.

Secondly, we suppose that $\beta_i > 0$ and $\beta_j > \beta_k > 0$. Then, from (4.62), it follows that $\beta_i > \beta_j$, and $\beta_i > \beta_k + \alpha_k\beta_k/2 > \beta_k$ since $0 < \alpha_k < 2$. The condition that $\beta_i > \beta_j$ and $\beta_i > \beta_k$ ensures that the first vertical asymptotes of $\mathcal{B}_{\text{new}}(\zeta)$ and $\mathcal{B}_{\text{old}}(\zeta)$ must satisfy $\mu_{\text{m}}^{\text{new}} \ge \mu_{\text{m}}^{\text{old}}$. Furthermore, it follows from (C.12 *b*) that $\mathcal{B}_{\text{new}}(\zeta) < \mathcal{B}_{\text{old}}(\zeta)$ on $0 < \zeta < \mu_{\text{m}}^{\text{old}}$. Consequently, Case II of the Lemma yields that $\mu_0^{\text{old}} < \mu_0^{\text{new}}$. This establishes the second statement of Qualitative Result III.

Finally, we suppose that $\beta_j < 0$, $\beta_k > 0$, and $\beta_i = \beta_j + \alpha_k\beta_k/2 < 0$. Then, since $\beta_i < 0$, it follows that the first vertical asymptote $\mu_{\text{m}}^{\text{old}}$ for $\mathcal{B}_{\text{old}}(\zeta)$ cannot occur from the i^{th} patch. The condition $\beta_k > 0$ then ensures that $\mu_{\text{m}}^{\text{new}} \le \mu_{\text{m}}^{\text{old}}$, where $\mu_{\text{m}}^{\text{new}}$ is the vertical asymptote of $\mathcal{B}_{\text{new}}(\zeta)$. Furthermore, it follows from (C.12 *a*) that $\mathcal{B}_{\text{new}}(\zeta) > \mathcal{B}_{\text{old}}(\zeta)$ on $0 < \zeta < \mu_{\text{m}}^{\text{new}}$. Consequently, Case I of the Lemma establishes that $\mu_0^{\text{old}} < \mu_0^{\text{new}}$, which proves the final statement of Qualitative Result III. ■

As a remark, we now give an interpretation of the first statement of Qualitative Result III in terms of the areas of the patches for the special case where $m_j = m_k = 1$. Then, from (4.63) it follows that the fragmentation of a favorable interior habitat is advantageous when the area $\varepsilon^2 A_k \equiv \pi\varepsilon^2\rho_k^2/2$ of a new favorable habitat centered at a smooth point of the boundary is at least twice as large as the area $\varepsilon^2 A_j \equiv \pi\varepsilon^2\rho_j^2$ of the new smaller favorable interior habitat. If the new boundary habit is located at a $\pi/2$ corner of the domain, for which $\alpha_k = 1/2$, then a sufficient condition for this fragmentation to be advantageous is when the area ratio satisfies $A_k/A_j = \rho_k^2/(4\rho_j^2) > 2/3$.

Acknowledgements

The notes herein are to a very large extent based on many joint projects with various collaborators and former graduate students of mine. In this regard, I very gratefully acknolwedge the important contributions of W. Chen, A. Cheviakov, D. Coombs, J. B. Keller, T. Kolokolnikov, M. C. Kropinski, A. Lindsay, A. Peirce, S. Pillay, R. Spiteri,

R. Straube, M. Titcombe, and J. Wei, to these notes. M. J. W. also acknowledges the grant support of NSERC (Canada).

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