An Asymptotic Analysis of the Mean First Passage Time for Narrow Escape Problems: Part II: The Sphere

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The mean first passage time (MFPT) is calculated for a Brownian particle in a spherical domain in \( \mathbb{R}^3 \) that contains \( N \) small non-overlapping absorbing windows, or traps, on its boundary. For the unit sphere, the method of matched asymptotic expansions is used to derive an explicit three-term asymptotic expansion for the MFPT for the case of \( N \) small locally circular absorbing windows. The third term in this expansion, not previously calculated, depends explicitly on the spatial configuration of the absorbing windows on the boundary of the sphere. The three-term asymptotic expansion for the average MFPT is shown to be in very close agreement with full numerical results. The average MFPT is shown to be minimized for trap configurations that minimize a certain discrete variational problem. This variational problem is closely related to the well-known optimization problem of determining the minimum energy configuration for \( N \) repelling point charges on the unit sphere. Numerical results, based on global optimization methods, are given for the optimum arrangements of the centers \( \{x_1, \ldots, x_N\} \) of \( N \) circular traps on the boundary of the sphere. These optimum arrangements are compared with corresponding results for the classical Coulomb or logarithmic discrete energy functions.

Key words: Narrow Escape, Mean First Passage Time (MFPT), Matched Asymptotic Expansions, Surface Neumann Green’s Functions, Discrete Variational Problem, Logarithmic Switchback Terms.

1 Introduction

The narrow escape problem concerns the motion of a Brownian particle confined in a bounded domain \( \Omega \subset \mathbb{R}^d \) (\( d = 2, 3 \)) 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 \( \tau \) taken for the Brownian particle to become absorbed somewhere in \( \partial \Omega_a \) starting initially from \( X(0) = x \in \Omega \), so that \( v(x) = E[\tau \mid X(0) = x] \). The calculation of \( v(x) \) becomes a narrow escape problem in the limit when the measure of the absorbing set \( |\partial \Omega_a| = O(\varepsilon^{d-1}) \) 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.

The narrow escape problem has many applications in biophysical modeling (see \[2\], \[16\], \[19\], \[38\], and the references therein). For the case of a two-dimensional domain, the narrow escape problem has been studied with a variety of analytical methods in \[19\], \[41\], \[42\], \[20\], and in the companion paper \[29\]. In this paper, we use the method of matched asymptotic expansions to study the narrow escape problem in a certain three-dimensional context.

In a three-dimensional bounded domain \( \Omega \), it is well-known (cf. \[19\], \[34\], \[37\]) that the MFPT \( v(x) \) satisfies a
Poisson equation with mixed Dirichlet-Neumann boundary conditions, formulated as

\begin{align}
\Delta v &= -\frac{1}{D}, \quad x \in \Omega; \\
v &= 0, \quad x \in \partial\Omega_a = \bigcup_{j=1}^{N} \partial\Omega_{\xi_j}, \quad j = 1, \ldots, N; \\
\partial_n v &= 0, \quad x \in \partial\Omega_r. 
\end{align}

(1.1)

Here $D$ is the diffusivity of the underlying Brownian motion, and the absorbing set consists of $N$ small disjoint absorbing windows, or traps, $\partial\Omega_{\xi_j}$ for $j = 1, \ldots, N$ each of area $|\partial\Omega_{\xi_j}| = \mathcal{O}(\varepsilon^2)$. We assume that $\partial\Omega_{\xi_j} \to x_j$ 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

\begin{align}
\bar{v} = \chi \equiv \frac{1}{|\Omega|} \int_{\Omega} v(x) \, dx,
\end{align}

(1.2)

where $|\Omega|$ is the volume of $\Omega$. The geometry of a confining sphere with traps on its boundary is depicted in Fig. 1.

Figure 1. 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 (1.1), for a bounded three-dimensional domain. For the case of one locally circular absorbing window of radius $\varepsilon$ on the boundary of the unit sphere, it was shown in [40] (with a correction as noted in [43]) that a two-term expansion for the average MFPT is given by

\begin{align}
\bar{v} \sim \frac{|\Omega|}{4\varepsilon D} \left[ 1 - \frac{\varepsilon}{\pi} \log \varepsilon + \mathcal{O}(\varepsilon) \right],
\end{align}

(1.3)

where $|\Omega|$ denotes the volume of the unit sphere. This result was derived in [40] 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 [40] 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 $\varepsilon$ on its smooth boundary, it was shown in [43] that

\begin{align}
\bar{v} \sim \frac{|\Omega|}{4\varepsilon D} \left[ 1 - \frac{\varepsilon}{H} \log \varepsilon + \mathcal{O}(\varepsilon) \right],
\end{align}

(1.4)

where $H$ denotes the mean curvature of the domain boundary at the center of the absorbing window. In [20] 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 unspecified $\mathcal{O}(1)$ term, which was estimated from Brownian particle simulations.
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The primary goal of this paper is to extend the previous work by calculating 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 will show 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 \( |x_i - x_j| = O(1) \) for \( i \neq j \), our results in §2 show that the average MFPT has the three-term asymptotic expansion

\[
\bar{v} = \frac{|S|}{4\pi DN} \left[ 1 + \frac{\varepsilon}{\pi} \log \left( \frac{2}{\varepsilon} \right) + \frac{\varepsilon}{\pi} \left( -\frac{9N}{5} + 2(N-2) \log 2 + \frac{3}{2} + \frac{4}{N} \mathcal{H}(x_1, \ldots, x_N) \right) + O(\varepsilon^2 \log \varepsilon) \right], \tag{1.5 a}
\]

where the discrete energy-like function \( \mathcal{H}(x_1, \ldots, x_N) \) is defined by

\[
\mathcal{H}(x_1, \ldots, x_N) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \left( \frac{1}{|x_i - x_j|} - \frac{1}{2} \log |x_i - x_j| - \frac{1}{2} \log (2 + |x_i - x_j|) \right). \tag{1.5 b}
\]

Results from (1.5) are shown in §2 to agree very closely with full numerical results computed with the finite element package COMSOL [6]. In §2 a corresponding three-term result is then given for the case of \( N \) arbitrarily-shaped, well-separated, windows on the boundary of the unit sphere.

The asymptotic analysis in §2 leading to (1.5), and related results, 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. This calculation is done in Appendix A. The identification of a weak logarithmic singularity for this Green’s function was first made in [23] for the unit sphere, and for a general three-dimensional domain in [31], [39], and [43]. Secondly, the analysis in §2 requires the introduction of certain logarithmic switchback terms that commonly occur in the asymptotic analysis of certain problems in fluid mechanics (see [26] and [27] for a discussion of logarithmic switchback terms).

In §3 we use the method of matched asymptotic expansions to derive a three-term asymptotic expansion for the principal eigenvalue \( \lambda(\varepsilon) \) of the Laplacian in the unit sphere for the case where the boundary of the sphere has \( N \) locally circular well-separated traps of small radii. This analysis extends the leading-order asymptotic calculation of [45]. Our results show that, to within the three-term asymptotic approximation, the principal eigenvalue \( \lambda(\varepsilon) \) is related to the average MFPT \( \bar{v} \) by \( \lambda \sim 1/(D\bar{v}) \). Related eigenvalue perturbation and optimization problems for the Laplacian in two-dimensional domains with localized interior traps, or with traps on the domain boundary, are studied in [4], [7], [8], [9], and [24] (see also the references therein).

For the case of \( N \) locally circular windows of a common radius, the discrete energy \( \mathcal{H}(x_1, \ldots, x_N) \) in (1.5) shows explicitly the dependence on the MFPT of the spatial arrangement of the absorbing windows. From (1.5), the average MFPT \( \bar{v} \) is minimized, and the corresponding principal eigenvalue of the Laplacian maximized, at the trap configuration \( \{x_1, \ldots, x_N\} \) that minimizes \( \mathcal{H}(x_1, \ldots, x_N) \). This discrete variational problem is an extension of the well-known problem of finding the minimum energy configuration of \( N \) repelling point charges on the surface of the unit sphere (see [32], [33], and the references therein). In §4 global optimization methods methods are used to obtain numerical results for the trap configurations \( \{x_1, \ldots, x_N\} \) that minimize \( \bar{v} \), and the results are compared with corresponding optimal configurations for two classical discrete energy functions; the logarithmic energy and the Coulomb energy. Moreover, a scaling law, with coefficients fitted to the numerical data, is derived to predict the minimum of the discrete energy \( \mathcal{H}(x_1, \ldots, x_N) \) in the limit \( N \to \infty \).

Finally, some open problems are suggested in §5.
In this section we asymptotically calculate the MFPT for escape from the unit sphere when 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 \( \varepsilon a_j \) where \( \varepsilon \ll 1 \). The problem for the MFPT \( v = v(x) \), written in spherical coordinates, is

\[
\begin{align*}
\Delta v &\equiv v_{rr} + \frac{2}{r} v_r + \frac{1}{r^2 \sin^2 \theta} v_{\phi \phi} + \frac{\cot \theta}{r^2} v_\theta + \frac{1}{r^2 v_{\theta \theta}} = -\frac{1}{D}, & r = |x| \leq 1, \\
v &\equiv 0, & x \in \partial \Omega, = \bigcup_{j=1}^N \partial \Omega_{x_j}, & j = 1, \ldots, N; \\
\partial_r v &\equiv 0, & x \in \partial \Omega \setminus \partial \Omega.
\end{align*}
\]

(2.1a)

(2.1b)

Here each \( \partial \Omega_{x_j} \) for \( j = 1, \ldots, N \) is a small “circular” cap centered at \((\theta_j, \phi_j)\) defined by

\[
\partial \Omega_{x_j} = \{(\theta, \phi) \mid (\theta - \theta_j)^2 + \sin^2(\theta_j)(\phi - \phi_j)^2 \leq \varepsilon^2 a_j^2\}.
\]

(2.1c)

The area of \( \partial \Omega_{x_j} \) is \(|\partial \Omega_{x_j}| \sim \pi \varepsilon^2 a_j^2\). In (2.1a), \( 0 \leq \phi \leq 2\pi \) 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 (2.1) asymptotically, we first must calculate the surface Neumann Green’s function. For the unit sphere \( \Omega \) with volume \(|\Omega| = 4\pi/3\), the surface Neumann Green’s function \( G_s(x; x_j) \) satisfies

\[
\begin{align*}
\Delta G_s &\equiv \frac{1}{|\Omega|}, & x \in \Omega; \\
\partial_r G_s &\equiv \delta(\cos \theta - \cos \theta_j)\delta(\phi - \phi_j), & x \in \partial \Omega; \\
\int_{\Omega} G_s \, dx &\equiv 0.
\end{align*}
\]

(2.2)

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

\[
x = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta), \\
x_j = (\cos \phi_j \sin \theta_j, \sin \phi_j \sin \theta_j, \cos \theta_j), \\
\gamma = x \cdot x_j,
\]

(2.3)

where \( \gamma \) 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 below in Appendix A.

**Lemma 2.1:** For the unit sphere, the surface Neumann Green’s function satisfying (2.2) is given explicitly by

\[
G_s(x; x_j) = \frac{1}{2\pi |x - x_j|} + \frac{1}{8\pi} \left(|x|^{-2} + 1\right) + \frac{1}{4\pi} \log \left(\frac{2}{1 - |x| \cos \gamma + |x - x_j|}\right) - \frac{7}{10\pi}.
\]

(2.4)

The calculations below for the MFPT require the limiting behavior of \( G_s \) in (2.4) as \( x \rightarrow x_j \in \partial \Omega \) when expressed in terms of a local coordinate system \((\eta, s_1, s_2)\) 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 \( \eta, s_1, \) and \( s_2 \) by

\[
y = \varepsilon^{-1}(x - x_j), \\
\eta = \varepsilon^{-1}(1 - r), \\
s_1 = \varepsilon^{-1}(\sin(\theta_j)(\phi - \phi_j)), \\
s_2 = \varepsilon^{-1}(\theta - \theta_j).
\]

(2.5)

From the law of cosines we calculate that

\[
1 - |x| \cos \gamma = \frac{1}{2} \left(|x - x_j|^2 - (|x|^2 - 1)\right) \sim \frac{1}{2} \left(\mathcal{O}(\varepsilon^2) - ((1 - \varepsilon\eta)^2 - 1)\right) \sim \varepsilon \eta + \mathcal{O}(\varepsilon^2).
\]

(2.6)

Therefore, upon substituting (2.6) and (2.5) into (2.4), we obtain as \( x \rightarrow x_j \) that

\[
G_s(x; x_j) = \frac{1}{2\pi \varepsilon |y|} - \frac{1}{4\pi} \log \left(\frac{\varepsilon}{2}\right) - \frac{1}{4\pi} \log (|y| + \eta) - \frac{9}{20\pi} + \mathcal{O}(\varepsilon).
\]

(2.7)

The weak logarithmic singularity in (2.7) on \( \eta = 0 \) was observed previously for the sphere in [23] (see page 247 of [23]), and for general domains in [39], [31], and [43]. Our calculation in Appendix A has identified the regular part of the singularity structure for \( G_s \) in (2.7), 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
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calculation, which we omit, shows that for \( x \to x_j \)
\[
\frac{1}{|y|} = \frac{1}{\rho} + \frac{\varepsilon}{2\rho^3} \left[ \eta(s_j^1 + s_j^2) - s_j^1 s_j^2 \cot \theta_j \right] + \mathcal{O}(\varepsilon^2), \quad \rho \equiv (\eta^2 + s_j^1 + s_j^2)^{1/2}.
\] (2.8)

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 (2.8) into (2.7) to obtain for \( x \to x_j \) that
\[
G_s(x; x_j) = \frac{1}{2\pi\varepsilon \rho} - \frac{1}{4\pi} \log \left( \frac{\varepsilon}{2} \right) + \frac{1}{4\pi} \left[ \frac{\eta(s_j^1 + s_j^2)}{\rho^3} - \frac{s_j^1 s_j^2 \cot \theta_j}{\rho^3} \right] - \frac{1}{4\pi} \log (\rho + \eta) - \frac{9}{20\pi} + \mathcal{O}(\varepsilon).
\] (2.9)

We now solve (2.1) 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
\[
v \sim \varepsilon^{-1} v_0 + v_1 + \varepsilon \log \left( \frac{\varepsilon}{2} \right) v_2 + \varepsilon v_3 + \cdots .
\] (2.10)

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 \( \varepsilon \) in (2.10) arises as a result of the term in (2.9) with logarithmic dependence on \( \varepsilon \). 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 (2.10), where \( \chi_0 \) 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. \[26, 27\]).

We first substitute (2.10) into (2.1) to obtain that \( v_k \), for \( k = 1, \ldots, 3 \), satisfies
\[
\Delta v_k = -\frac{1}{D} \delta_{k1} , \quad x \in \Omega; \quad \partial_n v_k = 0 , \quad x \in \partial \Omega \setminus \{ x_1 , \ldots , x_N \} ,
\] (2.11)

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 \( (\eta, s_1, s_2) \) as defined in (2.5), and we pose the inner expansion
\[
v \sim \varepsilon^{-1} w_0 + \log \left( \frac{\varepsilon}{2} \right) w_1 + w_2 + \cdots .
\] (2.12)

We substitute (2.12) into (2.1) after first transforming (2.1a) in terms of the local coordinate system (2.5) 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
\[
\mathcal{L} w_k \equiv w_{k\eta} + w_{k s_1 s_1} + w_{k s_2 s_2} = \delta_{k2} \mathcal{F}_2 , \quad \eta \geq 0 , \quad -\infty < s_1, s_2 < \infty ,
\] (2.13a)
\[
\partial_\eta w_k = 0 , \quad \text{on} \quad \eta = 0 , \quad s_1^2 + s_2^2 \geq a_j^2 ; \quad w_k = 0 , \quad \text{on} \quad \eta = 0 , \quad s_1^2 + s_2^2 \leq a_j^2 ,
\] (2.13b)

where \( \delta_{22} = 1 \) and \( \delta_{k2} = 0 \) if \( k = 0, 1 \). In (2.13a) \( \mathcal{F}_2 \), is defined by
\[
\mathcal{F}_2 \equiv 2 (\eta w_{0\eta} + w_{00}) - \cot \theta_j (w_{0 s_2} - 2 s_2 w_{0 s_1 s_1}) , \quad \eta \geq 0 , \quad -\infty < s_1, s_2 < \infty .
\] (2.13c)

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
\[
w_0 = v_0 (1 - w_c) ,
\] (2.14)

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
\[
\mathcal{L} w_c = 0 , \quad \eta \geq 0 , \quad -\infty < s_1, s_2 < \infty ,
\] (2.15a)
\[
\partial_\eta w_c = 0 , \quad \text{on} \quad \eta = 0 , \quad s_1^2 + s_2^2 \geq a_j^2 ; \quad w_c = 1 , \quad \text{on} \quad \eta = 0 , \quad s_1^2 + s_2^2 \leq a_j^2 .
\] (2.15b)
This is the well-known electrified disk problem in electrostatics (cf. [22]), whose solution is (see page 38 of [12])

\[
w_c = \frac{2}{\pi} \int_0^\infty \frac{\sin \mu}{\mu} e^{-\mu \eta/a_j} J_0 \left( \frac{\mu a_j}{L} \right) d\mu = \frac{2}{\pi} \sin^{-1} \left( \frac{a_j}{L} \right), \quad \sigma \equiv (s_j^2 + s_2^2)^{1/2},
\]

where \(J_0(z)\) is the Bessel function of the first kind of order zero, and \(L = L(\eta, \sigma)\) is defined by

\[
L(\eta, \sigma) \equiv \frac{1}{2} \left( [(\sigma + a_j)^2 + \eta^2]^{1/2} + [(\sigma - a_j)^2 + \eta^2]^{1/2} \right).
\]

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 (2.16a), we readily obtain the far-field behavior

\[
w_c \sim \frac{2a_j}{\pi} \left( \frac{1}{\rho} + \frac{a_j^2}{6} \left( \frac{1}{\rho^3} - \frac{3\eta^2}{\rho^3} \right) + \cdots \right), \quad \text{as} \quad \rho \to \infty,
\]

which is uniformly valid in \(\eta, s_1, \text{and} \ s_2\). Therefore, from (2.14) and (2.17), the far-field expansion for \(w_0\) is

\[
w_0 \sim v_0 \left( 1 - \frac{c_j}{\rho} + O(\rho^{-3}) \right), \quad \text{as} \quad \rho \to \infty, \quad c_j = \frac{2a_j}{\pi},
\]

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 (2.10) must agree with the far-field behavior of the inner expansion (2.12), so that

\[
\frac{v_0}{\varepsilon} + v_1 + \varepsilon \log \left( \frac{\varepsilon}{2} \right) v_2 + \varepsilon v_3 + \cdots \sim \frac{v_0}{\varepsilon} \left( 1 - \frac{c_j}{\rho} \right) + \log \left( \frac{\varepsilon}{2} \right) w_1 + w_2 + \cdots.
\]

Therefore, since \(\rho \sim \varepsilon^{-1}|x - x_j|\), we obtain that \(v_1\) must satisfy (2.11) 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

\[
\Delta v_1 = -\frac{1}{D}, \quad x \in \Omega; \quad \partial v_1 |_{x=1} = -2\pi v_0 \sum_{j=1}^N c_j \sin \theta_j \delta(\theta - \theta_j) \delta(\phi - \phi_j).
\]

By applying the divergence theorem, (2.20) has a solution only when \(v_0\) is given by

\[
v_0 = \frac{\left|\Omega\right|}{2\pi D N \varepsilon}, \quad \tilde{c} \equiv \frac{1}{N} \sum_{j=1}^N c_j, \quad c_j = \frac{2a_j}{\pi}.
\]

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 (2.20) 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 \(\chi\), as

\[
v_1 = -2\pi v_0 \sum_{i=1}^N c_i G_s(x; x_i) + \chi, \quad \chi \equiv \left|\Omega\right|^{-1} \int_{\Omega} v_1 \, dx.
\]

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 (2.9). Upon substituting the resulting expression into the matching condition (2.19) we obtain

\[
\frac{v_0}{\varepsilon} \left( 1 - \frac{c_j}{\rho} \right) + \frac{v_0 c_j}{2} \log \left( \frac{\varepsilon}{2} \right) + \chi + \frac{v_0 c_j}{2} \left[ \log(\eta + \rho) - \frac{\eta(s_1^2 + s_2^2)}{\rho^3} + \frac{s_1^2 s_2 \cot \theta_j}{\rho^3} \right] + B_j
\]

\[
+ \varepsilon \log \left( \frac{\varepsilon}{2} \right) v_2 + \varepsilon v_3 + \cdots \sim \frac{v_0}{\varepsilon} \left( 1 - \frac{c_j}{\rho} + O(\rho^{-3}) \right) + \log \left( \frac{\varepsilon}{2} \right) w_1 + w_2 + \cdots.
\]
Here the constant $B_j$ is defined by

$$B_j = -2\pi v_0 \left( -\frac{9}{20\pi} c_j + \sum_{i=1}^{N} c_i G_{sji} \right), \quad G_{sji} = G_s(x_j; x_i). \quad (2.24)$$

We compare the $O(\log \varepsilon)$ terms on both sides of (2.23), 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 $\chi$ in the form

$$\chi = \log \left( \frac{\varepsilon}{\beta} \right) \chi_0 + \chi_1, \quad (2.25)$$

where $\chi_0$ and $\chi_1$ are constants, independent of $\varepsilon$, to be found. This choice for $\chi$ is equivalent to inserting a constant term of order $O(\log \varepsilon)$ between $v_0$ and $v_1$ in the outer expansion (2.10). With this choice of $\chi$ in (2.23), the matching condition (2.23) enforces that $w_1 \sim \chi_0 + v_0 c_j / 2$ as $\rho \to \infty$. The solution $w_1$ to (2.13) that satisfies this far-field behavior is

$$w_1 = \left( \frac{v_0 c_j}{2} + \chi_0 \right) (1 - w_c), \quad (2.26)$$

where $w_c$, given explicitly in (2.16), is the solution to (2.15). Therefore, using (2.17), we obtain the far-field behavior

$$w_1 \sim \left( \frac{v_0 c_j}{2} + \chi_0 \right) \left( 1 - \frac{c_j}{\rho} + O(\rho^{-3}) \right). \quad (2.27)$$

Next, we substitute (2.27) into the matching condition (2.23) and use $\rho \sim \varepsilon^{-1} |x - x_0|$. This yields that the solution $v_2$ to (2.11) has the singular behavior $v_2 \sim - (v_0 c_j / 2 + \chi_0) c_j / |x - x_j|$ as $x \to x_j$. Therefore, $v_2$ satisfies

$$\Delta v_2 = 0, \quad x \in \Omega; \quad \partial_r v_2 |_{r=1} = -2\pi \sum_{j=1}^{N} c_j \left( \frac{v_0 c_j}{2} + \chi_0 \right) \frac{\delta(\theta - \theta_j) \delta(\phi - \phi_j)}{\sin \theta_j}. \quad (2.28)$$

By using the divergence theorem, we obtain that (2.28) is solvable only when $\chi_0$ is given by

$$\chi_0 = -\frac{v_0}{2N} \sum_{j=1}^{N} c_j^2. \quad (2.29)$$

Then, the solution for $v_2$ can be written in terms of the surface Neumann Green’s function as

$$v_2 = -2\pi \sum_{i=1}^{N} c_i \left( \frac{v_0 c_i}{2} + \chi_0 \right) G_s(x; x_i) + \chi_2. \quad (2.30)$$

Next, we match the $O(1)$ terms in (2.23) with $\chi$ as given in (2.25). We obtain that $w_2$ satisfies (2.13) with the far-field behavior

$$w_2 \sim B_j + \chi_1 + \frac{v_0 c_j}{2} \left[ \log(\eta + \rho) - \frac{\eta(s_1^2 + s_2^2)}{\rho^3} \right] + \left( \frac{v_0 c_j}{2\rho^3} \right) s_1^2 s_2 \cot \theta_j, \quad \text{as} \quad \rho \to \infty. \quad (2.31)$$

By superposition, we decompose the solution to this problem for $w_2$ in the form

$$w_2 = (B_j + \chi_1) (1 - w_c) + v_0 w_{2c} + v_0 w_{2c}^0, \quad (2.32)$$

where $w_c$ is the solution to the electrified disk problem (2.15). Upon writing $w_0 = v_0 (1 - w_c)$ to calculate $\mathcal{F}_2$ in (2.13c), we set $w_{2c}$ to be the solution to

$$w_{2c} \sim c_j \frac{1}{2} \log(\eta + \rho) - \frac{c_j}{2\rho^3} \eta(s_1^2 + s_2^2), \quad \text{as} \quad \rho \to \infty. \quad (2.33c)$$
Moreover, \( w_{2e} \) is taken to be the solution of

\[
\begin{align*}
&w_{2o\alpha} + w_{2o s_1} + w_{2o s_2} = \cot \theta_j (w_{cs_2} - 2s_2 w_{cs_1}s_1), \quad \eta \geq 0, \quad -\infty < s_1, s_2 < \infty, \tag{2.34 a} \\
&\partial_\eta w_{2o} = 0, \quad \text{on} \quad \eta = 0, \quad s_1^2 + s_2^2 \geq a_j^2; \quad w_{2o} = 0, \quad \text{on} \quad \eta = 0, \quad s_1^2 + s_2^2 \leq a_j^2, \tag{2.34 b} \\
&w_{2o} \sim \frac{c_j}{2\rho^3} s_1^2 s_2 \cot \theta_j, \quad \text{as} \quad \rho \to \infty. \tag{2.34 c}
\end{align*}
\]

In Appendix B we show that the inhomogeneous terms given by the right-hand sides of (2.33 a) and (2.34 a) lead explicitly to the leading-order far-field asymptotic behavior as written in (2.33 c) and (2.34 c).

The solution \( v_1 \) in (2.22) involves an as yet unknown constant \( \chi_1 \) from (2.25). In the determination of \( \chi_1 \) below from a solvability condition applied to the problem for \( v_3 \), we must have identified all of the monopole terms of the form \( b/\rho \) as \( \rho \to \infty \) for some constant \( b \) arising from the far-field behavior of each term in the decomposition (2.32) of \( w_2 \). It is only these monopole terms that give non-vanishing contributions in the solvability condition determining \( \chi_1 \). Clearly, the first term \( (B_j + \chi_1)(1 - w_c) \) in (2.32) yields a monopole term from (2.17). However, upon solving the problem for \( w_{2e} \) exactly as in Lemma B.1 of Appendix B, we obtain that \( w_{2e} \) also yields a monopole term, and it has the far-field behavior

\[
w_{2e} = \frac{c_j}{2} \log(\eta + \rho) - \frac{c_j}{2\rho^3} \eta(s_1^2 + s_2^2) - \frac{c_j k_j}{\rho} + \mathcal{O}(\rho^{-2}), \quad \text{as} \quad \rho \to \infty, \tag{2.35}
\]

where \( k_j \) is given explicitly by

\[
k_j = \frac{c_j}{2} \left[ 2 \log 2 - \frac{3}{2} + \log a_j \right]. \tag{2.36}
\]

Alternatively, the solution \( w_{2o} \) to (2.34) 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.

In this way, we obtain that the solution \( w_2 \) to (2.13) with leading-order far-field behavior (2.31) generates further terms in the far-field behavior of the form

\[
w_2 \sim (B_j + \chi_1) \left( 1 - \frac{c_j}{\rho} \right) + \frac{v_0 c_j}{2} \left[ \log(\eta + \rho) - \frac{\eta}{\rho^3} (s_1^2 + s_2^2) + \frac{s_1^2 s_2}{\rho^5} \cot \theta_j - \frac{2k_j}{\rho} + \mathcal{O}(\rho^{-2}) \right], \quad \text{as} \quad \rho \to \infty. \tag{2.37}
\]

Finally, we substitute (2.37) into the matching condition (2.23). The two monopole terms in (2.37) determine the singular behavior for the solution \( v_3 \) of (2.11) as

\[
v_3 \sim -\frac{c_j (B_j + \chi_1 + v_0 k_j)}{|x - x_j|} \quad \text{as} \quad x \to x_j. \tag{2.38}
\]

In distributional form, this problem for \( v_3 \) is equivalent to

\[
\Delta v_3 = 0, \quad x \in \Omega; \quad \partial_\nu v_3|_{\nu = 1} = -2\pi \sum_{j=1}^N c_j (B_j + \chi_1 + v_0 k_j) \frac{\delta(\theta - \theta_j) \delta(\phi - \phi_j)}{\sin \theta_j}. \tag{2.39}
\]

The solvability condition for (2.39), obtained by using the divergence theorem, determines \( \chi_1 \) as

\[
\chi_1 = -\frac{1}{N c} \sum_{j=1}^N c_j [B_j + v_0 k_j]. \tag{2.40}
\]

Then, upon using (2.24) for \( B_j \), we can write \( \chi_1 \) as the sum of two terms, one of which involves a quadratic form in terms of the capacitance vector \( \mathbf{C} = (c_1, \ldots, c_N) \), as

\[
\chi_1 = \frac{2\pi v_0}{N c} p_c(x_1, \ldots, x_N) - \frac{v_0}{N c} \sum_{j=1}^N c_j k_j, \quad p_c(x_1, \ldots, x_N) \equiv \mathbf{C} \mathbf{G}_s \mathbf{C}. \tag{2.41}
\]
Here $\kappa_j$ is given in (2.36) and $G_s$ is the Green’s function matrix defined in terms of $G_s(x_i; x_j)$ by

$$G_s = \begin{pmatrix} R & G_{s12} & \cdots & G_{s1N} \\ G_{s21} & R & \cdots & G_{s2N} \\ \vdots & \vdots & \ddots & \vdots \\ G_{sN1} & \cdots & \cdots & R \end{pmatrix}, \quad R = -\frac{9}{20\pi}, \quad G_{sij} = G_s(x_i; x_j). \quad (2.42)$$

Finally, we substitute (2.21) for $v_0$ together with (2.22) for $v_1$, with $\chi$ as determined by (2.25), (2.29), and (2.41), into the outer expansion (2.10). This leads to the following main result:

**Principal Result 2.2:** For $\varepsilon \to 0$, the asymptotic solution to (2.1) is given in the outer region $|x - x_j| \gg O(\varepsilon)$ for $j = 1, \ldots, N$ by

$$v = \frac{|\Omega|}{2\pi \varepsilon DNc} \left[ 1 + \varepsilon \log \left( \frac{2}{\varepsilon} \right) \frac{\sum_{j=1}^{N} c_j^2}{2Nc} + 2\pi \varepsilon \sum_{j=1}^{N} c_j G_s(x; x_j) + \frac{2\pi \varepsilon}{Nc} p_v(x_1, \ldots, x_N) - \frac{\varepsilon}{Nc} \sum_{j=1}^{N} c_j \kappa_j + O(\varepsilon^2 \log \varepsilon) \right]. \quad (2.43)$$

Here $c_j = 2a_j/\pi$ is the capacitance of the $j^{th}$ circular absorbing window of radius $a_j$, $\bar{v} \equiv N^{-1}(c_1 + \ldots + c_N)$, $|\Omega| = 4\pi^3/3$, $\kappa_j$ is defined in (2.36), $G_s(x; x_j)$ is the surface Neumann Green’s function given in (2.4), and $p_v(x_1, \ldots, x_N)$ is the quadratic form defined in (2.44). Since $\int_{\Omega} G_s \, dx = 0$, then $\bar{v} = |\Omega|^{-1} \int_{\Omega} v \, dx$ is given by

$$\bar{v} = \frac{|\Omega|}{2\pi \varepsilon DNc} \left[ 1 + \varepsilon \log \left( \frac{2}{\varepsilon} \right) \frac{\sum_{j=1}^{N} c_j^2}{2Nc} + 2\pi \varepsilon \sum_{j=1}^{N} c_j G_s(x; x_j) + \frac{2\pi \varepsilon}{Nc} p_v(x_1, \ldots, x_N) - \frac{\varepsilon}{Nc} \sum_{j=1}^{N} c_j \kappa_j + O(\varepsilon^2 \log \varepsilon) \right]. \quad (2.44)$$

For the case of one circular window of radius $\varepsilon a$, we set $N = 1$, $c_1 = 2a/\pi$, and $a_1 = a_i$ in (2.43), (2.36), and (2.44) to get

$$\bar{v} = \frac{|\Omega|}{4\varepsilon a D} \left[ 1 + \frac{\varepsilon a}{\pi} \log \left( \frac{2}{\varepsilon a} \right) + \frac{\varepsilon a}{\pi} \left( -\frac{9}{5} - 2 \log 2 + \frac{3}{2} \right) + O(\varepsilon^2 \log \varepsilon) \right], \quad v(x) = \bar{v} - \frac{|\Omega|}{D} G_s(x; x_1). \quad (2.45)$$

For an initial position at the origin, i.e. $x = (0, 0)$, then with $G_s(0; x_1) = -3/(40\pi)$ from (2.4), (2.45) becomes

$$v(0) = \frac{|\Omega|}{4\varepsilon a D} \left[ 1 + \frac{\varepsilon a}{\pi} \log \left( \frac{2}{\varepsilon a} \right) - \frac{2\varepsilon a \log 2}{\pi} + O(\varepsilon^2 \log \varepsilon) \right]. \quad (2.46)$$

For the case of one circular absorbing window of radius $\varepsilon$ (i.e. $a = 1$), it was derived in [40] that

$$\bar{v} \sim \frac{|\Omega|}{4\varepsilon D} \left[ 1 + \frac{\varepsilon}{\pi} \log \left( \frac{1}{\varepsilon} \right) + O(\varepsilon) \right]. \quad (2.47)$$

The original result in equation (3.52) of [40] omits the $\pi$ term in (2.47) due to an omission of an extra factor of $\pi$ on the left-hand side of the equation above (3.52) of [40]. This was corrected in [43]. Our result (2.45) agrees asymptotically with that of (2.47) and determines the $O(\varepsilon)$ term to $\bar{v}$ explicitly. More importantly, our main result in Principal Result 2.2 generalizes that of [40] to the case of $N$ circular absorbing windows of different radii on the unit sphere, and provides the $O(\varepsilon)$ term that accounts for the specific locations of the traps on the unit sphere.

A further interesting special case of Principal Result 2.2 is when there are $N$ circular absorbing windows of a common radius $\varepsilon$. Then, upon setting $c_j = 2/\pi$, together with $a_j = 1$ for $j = 1, \ldots, N$ in (2.36), (2.44) reduces to

$$\bar{v} = \frac{|\Omega|}{4\varepsilon DN} \left[ 1 + \frac{\varepsilon}{\pi} \log \left( \frac{2}{\varepsilon} \right) + \frac{\varepsilon}{\pi} \left( -\frac{9}{5} + \frac{8\pi}{5} \sum_{i=1}^{N} \sum_{j=i+1}^{N} G_s(x_i; x_j) - 2 \log 2 + \frac{3}{2} \right) + O(\varepsilon^2 \log \varepsilon) \right]. \quad (2.48)$$
From (2.4), we readily calculate the interaction term $G_s(x_i; x_j)$ in (2.48) as

$$G_s(x_i; x_j) = -\frac{9}{20 \pi} + \frac{1}{2 \pi} \left( \frac{1}{|x_i - x_j|} - \frac{1}{2} \log \left[ \sin^2 \left( \frac{\gamma_{ij}}{2} \right) + \sin \left( \frac{\gamma_{ij}}{2} \right) \right] \right), \quad \cos(\gamma_{ij}) = x_i \cdot x_j,$$

where $\gamma_{ij}$ denotes the angle between $x_i$ and $x_j$. Therefore, (2.48) becomes

$$\bar{v} = \frac{|\Omega|}{4 \pi DN} \left[ 1 + \frac{\varepsilon}{\pi} \log \left( \frac{2}{\varepsilon} \right) + \frac{\varepsilon}{\pi} \left( -9 N + 2 \log 2 + \frac{3}{2} + \frac{4}{N} \hat{\mathcal{H}}(x_1, \ldots, x_N) \right) + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right].$$

Equivalently, we can write $\bar{v}$ in the alternative form

$$\bar{v} = \frac{|\Omega|}{4 \pi DN} \left[ 1 + \frac{\varepsilon}{\pi} \log \left( \frac{2}{\varepsilon} \right) + \frac{\varepsilon}{\pi} \left( -9 N + 2(N - 2) \log 2 + \frac{3}{2} + \frac{4}{N} \mathcal{H}(x_1, \ldots, x_N) \right) + \mathcal{O}(\varepsilon^2 \log \varepsilon) \right],$$

where $\hat{\mathcal{H}}(x_1, \ldots, x_N)$ is defined by

$$\hat{\mathcal{H}}(x_1, \ldots, x_N) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \left( \frac{1}{|x_i - x_j|} - \frac{1}{2} \log |x_i - x_j| - \frac{1}{2} \log (2 + |x_i - x_j|) \right).$$

The first term in $\mathcal{H}$ is the usual Coulomb singularity in three-dimensions, whereas the second term in (2.51 b) represents a contribution from surface diffusion on the boundary of the sphere, similar to that studied in [7].

As a remark, for the case of $N$ circular absorbing windows of a common radius $\varepsilon$, 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 $\mathcal{H}(x_1, \ldots, x_N)$ on the unit sphere $|x_j| = 1$ for $j = 1, \ldots, N$. The classic discrete variational problems of minimizing either the Coulomb energy $\sum_{i=1}^{N} \sum_{j=i+1}^{N} |x_i - x_j|^{-1}$ or the logarithmic energy $-\sum_{i=1}^{N} \sum_{j=i+1}^{N} \log |x_i - x_j|$ on the unit sphere has a long history in approximation theory (see [11], [15], [3], [32], [33], [25], [17], and the references therein).

Next, we validate our asymptotic result (2.51) with full numerical results. In Fig. 2 we compare our asymptotic results for the average MFPT $\bar{v}$ versus $\varepsilon$ with those computed from full numerical simulations using the COMSOL.
Table 1. Comparison of asymptotic and full numerical results for $\bar{v}$ for either $N = 1$, $N = 2$, or $N = 4$, identical circular windows of radius $\varepsilon$ equidistantly placed on the surface of the unit sphere (see the caption of Fig. 2). Here $\bar{v}_2$ is the two-term asymptotic result obtained by omitting the $O(\varepsilon)$ term in (2.51), $\bar{v}_3$ is the three-term asymptotic result of (2.51), and $\bar{v}_n$ is the full numerical result computed from COMSOL [6].

finite element package [6]. 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. 2). Table 1 compares the two-term and three-term predictions for $\bar{v}$ from (2.51) with corresponding full numerical results computed using COMSOL. Note that the three-term expansion for $\bar{v}$ in (2.51) agrees well with full numerical results even when $\varepsilon = 0.5$. For $\varepsilon = 0.5$ and $N = 4$, we 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 1 show that the three-term asymptotic result for the average MFPT differs from the full numerical result by only about 10%.

Finally, we remark that our main result (2.44) can also readily be used for absorbing windows that are not circular. To treat this modification of (2.1), the following generalized electrified disk problem for $w_c$ replaces (2.15):

$$\begin{align*}
\mathcal{L}w_c &= 0, \quad \eta \geq 0, \quad -\infty < s_1, s_2 < \infty, \\
\partial_\eta w_c &= 0, \quad \text{on } \eta = 0, \quad (s_1, s_2) \notin \Omega; \quad w_c = 1, \quad \text{on } \eta = 0, \quad (s_1, s_2) \in \Omega, \\
w_c &\sim c_j/\rho, \quad \text{as } \rho \to \infty.
\end{align*}$$

Here the absorbing set $\Omega$ in the plane $\eta = 0$ is possibly multi-connected, which can incorporate the window clustering effect of [20]. When $\Omega$ has two lines of symmetry, then $w_c$ can be chosen to be even in $s_1$ and $s_2$, so that the far-field behavior of $w_c$ is $w_c \sim c_j/\rho + O(\rho^{-3})$ as $\rho \to \infty$, similar to that in (2.17). The analysis leading to (2.44) can then be repeated, and as remarked following (B.13) of Appendix B, the far-field behavior (2.37) will still hold for this generalized problem. Consequently, to treat the case of arbitrarily-shaped absorbing windows centered at $x_j$ for $j = 1, \ldots, N$ on the boundary of the unit sphere, we need only replace $c_j$ in (2.44) with the capacitance $c_j$ associated with the far-field behavior of (2.52). In addition, for an arbitrarily-shaped absorbing window, we must also re-calculate the monopole coefficient $\kappa_j$ in (2.44) from the solution to (B.4) subject to the far-field behavior (B.13). Although $c_j$ and $\kappa_j$ must in general be calculated numerically, such as from fast boundary integral methods of potential theory (cf. [44]), the capacitance $c_j$ is in fact known analytically for a few special geometries. In particular, for an elliptical-shaped absorbing window with semi-axes $a_j$ and $b_j$ so that $s_1^2/a_j^2 + s_2^2/b_j^2 = 1$ with $b_j < a_j$, then $c_j$ is given in terms of the complete elliptic integral of the first kind $K(\mu)$ as (see [40])

$$c_j = \frac{a_j}{K(c_j)}, \quad K(\mu) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - \mu^2 \sin^2 \theta}}, \quad e_j = \sqrt{1 - b_j^2/a_j^2}. \tag{2.53}$$

In addition, for the case of a cluster of two circular windows, each with radius $a_j$, and with center-to-center separation
Each boundary trap, average MFPT

Our asymptotic calculation will show, to within the three-term asymptotic approximation, that


c_j \sim \frac{4a_j}{\pi} \left[ 1 - \frac{a_j}{l\pi} + \frac{a_j^2}{l^2\pi^2} - \frac{a_j^3}{l^3\pi^3} + \cdots \right].

(2.54)

Upper and lower bounds for the capacitance $c_j$ of multiple non-overlapping circular disks are derived in [13]. Similar bounds are used in [20] to study the effect of window clustering on the average MFPT, whereby several circular absorbing windows are clustered within an $O(\varepsilon)$ region near some point on the boundary of the sphere. In our analysis, these bounds for the capacitance $c_j$ can be used in the three-term expansion (2.44) for the average MFPT.

3 The Principal Eigenvalue of the Laplacian

In this section we asymptotically calculate the principal eigenvalue of the Laplacian in the unit sphere $\Omega$, when the boundary of the sphere is almost entirely reflecting, but is perturbed by $N$ small non-overlapping locally circular absorbing traps $\partial \Omega_{\varepsilon,j}$, centered at $x_j$ with $|x_j| = 1$, for $j = 1, \ldots, N$. The perturbed eigenvalue problem is

\[
\Delta u = u_{rr} + \frac{2}{r} u_r + \frac{1}{r^2 \sin^2 \theta} u_{\phi \phi} + \cot \theta \frac{1}{r^2} u_\theta + \frac{1}{r^2} u_{\theta \theta} = -\lambda u, \quad x \in \Omega, \quad \int_\Omega u^2 \, dx = 1, \quad \partial_r u = 0, \quad x \in \partial \Omega \setminus \partial \Omega_\varepsilon; \quad u = 0, \quad x \in \partial \Omega_\varepsilon \equiv \bigcup_{j=1}^N \partial \Omega_{\varepsilon,j}. \tag{3.1a}
\]

Each boundary trap, $\partial \Omega_{\varepsilon,j}$ for $j = 1, \ldots, N$ is a small “circular” cap centered at $(\theta_j, \phi_j)$, as defined by (2.1 c), with area $|\partial \Omega_{\varepsilon,j}| \sim \pi \varepsilon^2 a_j^2$, and with $\partial \Omega_j \rightarrow x_j$ as $\varepsilon \to 0$, where $x_j = (\cos \phi_j \sin \theta_j, \sin \phi_j \sin \theta_j, \cos \theta_j)$. Here $0 \leq \phi \leq 2\pi$ is the longitude and $0 \leq \theta \leq \pi$ is the latitude.

We let $\lambda(\varepsilon)$ denote the principal eigenvalue of (3.1), with corresponding eigenfunction $u(x, \varepsilon)$. Clearly, $\lambda(\varepsilon) \to 0$ as $\varepsilon \to 0$ with $u \to u_0 = |\Omega|^{-1/2}$. A leading-order calculation for $\lambda(\varepsilon)$ was given in Section 5.2 of [45]. Here, we use a more refined matched asymptotic analysis to calculate a three-term asymptotic expansion for $\lambda(\varepsilon)$ as $\varepsilon \to 0$.

Our asymptotic calculation will show, to within the three-term asymptotic approximation, that $\lambda(\varepsilon)$ is related to the average MFPT $\tilde{v}$ of (1.2) by $\lambda \sim 1/(D\tilde{v})$.

We expand the principal eigenvalue for (3.1) as

\[
\lambda = \varepsilon \lambda_1 + \varepsilon^2 \log \left( \frac{\varepsilon}{2} \right) \lambda_2 + \varepsilon^2 \lambda_3 + \cdots. \tag{3.2}
\]

In the outer region away from the boundary traps we expand the outer solution as

\[
u \sim u_0 + \varepsilon u_1 + \varepsilon^2 \log \left( \frac{\varepsilon}{2} \right) u_2 + \varepsilon^2 u_3 + \cdots, \tag{3.3}
\]

where $u_0 \equiv |\Omega|^{-1/2}$. The logarithmic terms in (3.2) and (3.3) arise as a direct consequence of the subdominant logarithmic singularity of the surface Neumann Green’s function given in (2.7).

We first substitute (3.3) into (3.1) to obtain that $u_k$ for $k = 1, 2$ satisfies

\[
\Delta u_k = -\lambda_k u_0, \quad x \in \Omega; \quad \partial_r u_k = 0, \quad x \in \partial \Omega \setminus \{x_1, \ldots, x_N\}; \quad \int_\Omega u_k \, dx = 0. \tag{3.4}
\]

In contrast, $u_3$ satisfies

\[
\Delta u_3 = -\lambda_1 u_1 - \lambda_3 u_0, \quad x \in \Omega; \quad \partial_r u_3 = 0, \quad x \in \partial \Omega \setminus \{x_1, \ldots, x_N\}; \quad \int_\Omega (u_1^2 + 2u_0 u_3) \, dx = 0. \tag{3.5}
\]

In the inner region near the $j$th boundary trap we introduce the local coordinate system $(\eta, s_1, s_2)$ by (2.5). We
then write the inner expansion of the principal eigenfunction as
\[ u \sim w_0 + \varepsilon \log \left( \frac{\varepsilon}{2} \right) w_1 + \varepsilon w_2 + \cdots. \] (3.6)

We substitute (3.6) into (3.1) and then transform the Laplacian in (3.1) in terms of the local coordinate system (2.5). Upon collecting similar terms in \( \varepsilon \), we obtain that \( w_k \) for \( k = 0, 1, 2 \) satisfies (2.13).

The leading-order matching condition is that \( w_0 \sim w_0 = |\Omega|^{-1/2} \) as \( \rho \equiv (\eta^2 + s_1^2 + s_2^2)^{1/2} \to \infty \). Thus, we write
\[ w_0 = u_0 (1 - w_c), \] (3.7)
where \( w_c \) is the solution to the electrified disk problem (2.15), as given in (2.16). The far-field behavior of \( w_0 \) is given in (2.18). Upon writing (2.18) in terms of outer variables by using (2.5), we obtain the matching condition that the near-field behavior of the outer expansion (3.3) must agree with the far-field behavior of the inner expansion (3.6), so that
\[ u_0 + \varepsilon u_1 + \varepsilon^2 \log \left( \frac{\varepsilon}{2} \right) u_2 + \varepsilon^2 u_3 + \cdots \sim u_0 \left( 1 - \frac{c_j \varepsilon}{x - x_j} + \cdots \right) + \varepsilon \log \left( \frac{\varepsilon}{2} \right) w_1 + \varepsilon w_2 + \cdots. \] (3.8)

From this matching condition, we obtain that \( u_1 \) must satisfy (3.4) and have the singular behavior \( u_1 \sim -c_j u_0 / |x - x_j| \) as \( x \to x_j \) for \( j = 1, \ldots, N \). This problem can be written in distributional form as
\[ \Delta u_1 = -\lambda_1 u_0, \quad x \in \Omega; \quad \partial_r u_1 \big|_{r=1} = -2\pi u_0 \sum_{j=1}^{N} \frac{c_j}{\sin \theta_j} \delta(\theta - \theta_j)\delta(\phi - \phi_j), \] (3.9)
with \( \int_\Omega u_1 \, dx = 0 \). From the divergence theorem, and by using \( u_0 = |\Omega|^{-1/2} \), we calculate \( \lambda_1 \) as
\[ \lambda_1 = \frac{2\pi}{|\Omega|} \sum_{j=1}^{N} c_j, \quad c_j = \frac{2u_0}{\pi}. \] (3.10)

Then, the solution to (3.9) with \( \int_\Omega u_1 \, dx = 0 \) can be written as
\[ u_1 = -2\pi u_0 \sum_{i=1}^{N} c_i G_s(x; x_i). \] (3.11)

Here \( G_s(x; x_j) \) is the surface Neumann Green’s function satisfying (2.2). It is given explicitly in (2.4), and has the near-field behavior for \( x \to x_j \) as given in (2.9).

Next, we expand \( u_1 \) in (3.11) as \( x \to x_j \) by using the near-field behavior (2.9) for \( G_s \). Upon substituting the resulting expression into the matching condition (3.8), we obtain
\[ u_0 \left( 1 - \frac{c_j}{\rho} \right) + \frac{\varepsilon u_0 c_j}{2} \log \left( \frac{\varepsilon}{2} \right) - 2\varepsilon \pi u_0 B_j + \frac{\varepsilon u_0 c_j}{2} \left[ \log(\eta + \rho) - \frac{\eta (s_1^2 + s_2^2)}{\rho^3} + \frac{s_1^2 s_2 \cot \theta_j}{\rho^3} \right] \]
\[ + \varepsilon^2 \log \left( \frac{\varepsilon}{2} \right) u_2 + \varepsilon^2 u_3 + \cdots \sim u_0 \left( 1 - \frac{c_j}{\rho} \right) + \varepsilon \log \left( \frac{\varepsilon}{2} \right) w_1 + \varepsilon w_2 + \cdots. \] (3.12)

Here the constant \( B_j \) is defined by
\[ B_j = -\frac{9}{20\pi} c_j + \sum_{i=1}^{N} c_i G_{s_j,i}, \quad G_{s_j,i} \equiv G_s(x_j; x_i). \] (3.13)

The matching condition (3.12) for the \( \mathcal{O}(\varepsilon \log[\varepsilon/2]) \) terms yields that \( w_1 \sim c_j u_0 / 2 \) as \( \rho \to \infty \). The solution \( w_1 \) to (2.13) is given in terms of the solution \( w_c \) to (2.15) with far-field behavior (2.18), so that
\[ w_1 = \frac{c_j u_0}{2} (1 - w_c) \sim \frac{c_j u_0}{2} \left( 1 - \frac{c_j}{\rho} + \mathcal{O}(\rho^{-3}) \right), \quad \text{as} \ \rho \to \infty. \] (3.14)
Next, we substitute (3.14) into the matching condition (3.12) and use $\rho \sim \varepsilon^{-1}|x-x_0|$. By matching the $O(\varepsilon^2 \log \varepsilon)$ terms, we obtain that $u_2$ satisfies (3.4) with singular behavior $u_2 \sim -c_j^2 u_0/(2|x-x_j|)$ as $x \to x_j$ for $j = 1, \ldots, N$. Therefore, in distributional form, the problem for $u_2$ is equivalent to
\[
\Delta u_2 = -\lambda_2 u_0, \quad x \in \Omega; \quad \partial_r u_2|_{r=1} = -\pi u_0 \sum_{j=1}^{N} c_j^2 \frac{\delta(\theta - \theta_j)\delta(\phi - \phi_j)}{\sin \theta_j},
\]
with $\int_{\Omega} u_2 \, dx = 0$. From the divergence theorem, and by using $u_0 = |\Omega|^{-1/2}$, we calculate $\lambda_2$ as
\[
\lambda_2 = \frac{\pi}{|\Omega|} \sum_{j=1}^{N} c_j^2.
\]
Then, the solution $u_2$ to (3.15), with $\int_{\Omega} u_2 \, dx = 0$, is written in terms of $G_s(x;x_j)$ as
\[
u_2 = -\pi u_0 \sum_{j=1}^{N} c_j^2 G_s(x;x_j).
\]
Next, we match the $O(\varepsilon)$ terms on the left-hand side of (3.12). We obtain that $w_2$ satisfies the inhomogeneous problem (2.13), and has the far-field behavior
\[
w_2 \sim -2\pi u_0 B_j + \frac{c_j u_0}{2} \left[ \log(\eta + \rho) - \frac{\eta (s_1^2 + s_2^2)}{\rho^3} + \frac{s_1 s_2 \cot \theta_j}{\rho^3} \right], \quad \text{as} \quad \rho \to \infty.
\]
To determine $w_2$, we first set $w_0 = u_0(1 - w_c)$ in the definition of the inhomogeneous term $F_2$ in (2.13c), where $w_c$ is the solution to (2.15). Then, we decompose $w_2$ into the sum of three terms as
\[
w_2 = -2\pi B_j u_0 (1 - w_c) + u_0 w_{2c} + u_0 w_{2o}.
\]
With the operator $L$ as defined in (2.13a), $w_{2c}$ and $w_{2o}$ are the solutions of (2.33) and (2.34), respectively.

The explicit solution to (2.33) for $w_{2c}$ is given in Lemma B.1 of Appendix B. This solution has the far-field behavior (2.35). The explicit solution to (2.34) for $w_{2o}$ is given by Lemma B.2 of Appendix B. In this way, we obtain that $w_2$ has the far-field behavior
\[
w_2 \sim -2\pi B_j u_0 \left( 1 - \frac{c_j}{\rho} \right) + \frac{c_j u_0}{2} \left[ \log(\eta + \rho) - \frac{\eta (s_1^2 + s_2^2)}{\rho^3} - \frac{2\kappa_j}{\rho} \right] + \frac{c_j \eta}{2 \rho^3} (s_1^2 + s_2^2) + o(\rho^{-1}), \quad \text{as} \quad \rho \to \infty.
\]
By substituting (3.20) into the matching condition (3.12), we obtain that the two monopole terms in (3.20) proportional to $\rho^{-1}$ determine the singularity behavior for the correction term $u_3$ in (3.12). Therefore, we obtain that $u_3$ satisfies (3.5) with the singular behavior
\[
u_3 \sim \frac{2\pi B_j c_j u_0}{|x-x_j|} - \frac{c_j u_0 \kappa_j}{|x-x_j|}, \quad \text{as} \quad x \to x_j, \quad j = 1, \ldots, N,
\]
where $\kappa_j$ is defined in (2.36). This problem for $u_3$ can be written in distributional form as
\[
\Delta u_3 = -\lambda_1 u_1 - \lambda_3 u_0, \quad x \in \Omega; \quad \partial_r u_3|_{r=1} = u_0 \sum_{j=1}^{N} \left( 4\pi^2 B_j c_j - 2\pi c_j \kappa_j \right) \frac{\delta(\theta - \theta_j)\delta(\phi - \phi_j)}{\sin \theta_j}.
\]
By using the divergence theorem, together with $u_0 = |\Omega|^{-1/2}$, $\int_{\Omega} u_1 \, dx = 0$, and (2.36), we calculate $\lambda_3$ as
\[
\lambda_3 = -\frac{4\pi^2}{|\Omega|} \sum_{j=1}^{N} B_j c_j + \frac{\pi}{|\Omega|} \sum_{j=1}^{N} c_j^2 \left( 2 \log 2 - \frac{3}{2} + \log \eta_j \right).
\]
Finally, we substitute $u_0 = |\Omega|^{-1/2}$, (3.11), and (3.17), into (3.3) to obtain the outer expansion of the eigenfunction.
The perturbed eigenvalue is obtained by substituting (3.10), (3.16), and (3.23), into (3.2). We summarize the result as follows:

**Principal Result 3.1:** Consider (3.1) in the unit sphere $\Omega$ with $N$ small circular boundary traps of radius $\varepsilon a_j$ on $\partial \Omega$ centered at $x_j$ for $j = 1, \ldots, N$. Then, for $\varepsilon \to 0$, the asymptotic solution to (3.1) is given in the outer region $|x - x_j| \gg O(\varepsilon)$ for $j = 1, \ldots, N$ by

$$u = \frac{1}{|\Omega|^{1/2}} \left( 1 - 2\pi \varepsilon \sum_{j=1}^{N} c_j G(x; x_j) - \varepsilon^2 \pi \log \left( \frac{\varepsilon}{2} \right) \sum_{j=1}^{N} c_j^2 G(x; x_j) + O(\varepsilon^2) \right). \quad (3.24)$$

Here $c_j = 2a_j/\pi$ is the capacitance associated with the $j$th boundary trap of radius $\varepsilon a_j$, and $G(x; x_j)$ is the surface Neumann Green’s function given in (2.4). For $\varepsilon \to 0$, the principal eigenvalue $\lambda(\varepsilon)$ of (3.1) is given by

$$\lambda = \frac{2\pi \varepsilon N \bar{c}}{|\Omega|} + \frac{\pi \varepsilon^2}{|\Omega|} \sum_{j=1}^{N} c_j^2 \left( \log (\varepsilon a_j) + \log 2 - \frac{3}{2} \right) - \frac{4\pi \varepsilon^2}{|\Omega|} p_c(x_1, \ldots, x_N) + O(\varepsilon^3 \log \varepsilon), \quad (3.25a)$$

where $\bar{c} \equiv N^{-1} (c_1 + \ldots + c_N)$. The quadratic form $p_c(x_1, \ldots, x_N)$ in (3.25a) is defined in terms of the entries $G_{si,j}$ of the Green’s matrix $G$, of the form given in (2.4.2) by the weighted discrete sum

$$p_c(x_1, \ldots, x_N) \equiv \sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j G_{si,j}, \quad c_j = \frac{2a_j}{\pi}, \quad (3.25b)$$

where $G_{si,j} \equiv G(x_i; x_j)$ is given explicitly from (2.4) by

$$G_{si,j} = -\frac{9}{20\pi} + \frac{(1 - \delta_{ij})}{2\pi} \log (2 + \mathcal{H}_{si,j}), \quad i, j = 1, \ldots, N, \quad (3.25c)$$

$$\mathcal{H}_{si,j} = \frac{1}{|x_i - x_j|} - \frac{1}{2} \log |x_i - x_j| - \frac{1}{2} \log (2 + |x_i - x_j|), \quad i \neq j. \quad (3.25d)$$

Here $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$. In terms of $\mathcal{H}_{si,j}$, we can write (3.25a) as

$$\lambda = \frac{2\pi \varepsilon N \bar{c}}{|\Omega|} + \frac{\pi \varepsilon^2}{|\Omega|} \sum_{j=1}^{N} c_j^2 \left( \log (\varepsilon a_j) + 3 \log 2 - \frac{3}{2} \right) - \frac{4\pi \varepsilon^2}{|\Omega|} \sum_{i=1}^{N} \sum_{j=i+1}^{N} c_i c_j \mathcal{H}_{si,j} + \frac{\pi \varepsilon^2}{|\Omega|} \left( \frac{9}{5} - 2 \log 2 \right) \sum_{i=1}^{N} \sum_{j=1}^{N} c_i c_j + O(\varepsilon^3 \log \varepsilon). \quad (3.25e)$$

For the special case where there are $N$ identical circular boundary traps of a common radius $\varepsilon a$, then (3.25e) with $c = 2a/\pi$ and $|\Omega| = 4\pi/3$ reduces to

$$\lambda \sim \frac{2\pi \varepsilon N c}{|\Omega|} \left[ 1 + \frac{\varepsilon c}{2} \log (\varepsilon a) + \frac{\varepsilon c}{2} \left( \log 2 - \frac{3}{2} \right) + \frac{9\varepsilon c N}{10} - \varepsilon c (N - 1) \log 2 - \frac{2\varepsilon c}{N} \mathcal{H}(x_1, \ldots, x_N) \right]. \quad (3.26)$$

Here the discrete energy function $\mathcal{H}(x_1, \ldots, x_N) \equiv \sum_{i=1}^{N} \sum_{j=i+1}^{N} \mathcal{H}_{si,j}$ is given by (2.51b). For the case of one single trap, the result (3.26) yields the three-term expansion

$$\lambda \sim \frac{2\pi \varepsilon c}{|\Omega|} \left[ 1 + \frac{\varepsilon c}{2} \left( \log (\varepsilon a) + \log 2 - \frac{3}{2} \right) + \frac{9\varepsilon c}{10} \right]. \quad (3.27)$$

Upon setting $c = 2/\pi$ in (3.26), corresponding to $N$ locally circular traps of a common radius $\varepsilon$, it is readily verified from (3.26) and (2.51) that, to within the three-term asymptotic approximations, the relation $\hat{v} \sim 1/(\mathcal{D} \lambda)$ between the average MFPT and the principal eigenvalue is asymptotically valid in the limit $\varepsilon \to 0$. Therefore, we conclude that for the case of $N$ circular boundary traps of a common radius $\varepsilon a$, the principal eigenvalue of (3.1) is maximized,
and the corresponding MFPT minimized, in the limit $\varepsilon \to 0$ at the boundary trap configuration \{$x_1, \ldots, x_N$\} that minimizes the discrete sum $\mathcal{H}(x_1, \ldots, x_N)$ in (2.51b) on the unit sphere $|x_i| = 1$ for $j = 1, \ldots, N$.

4 Numerical Optimization Results for the Unit Sphere

Next, we numerically compute optimum arrangements \{\textit{x}_1, \ldots, \textit{x}_N\} of the centers of \textit{N} circular boundary traps of a common radius that minimizes the discrete energy (2.51b). We compare our results with corresponding optimal arrangements associated with minimizing either the Coulomb or logarithmic energies defined by

\[
\mathcal{H}_C = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{|x_i - x_j|}, \quad \mathcal{H}_L = -\sum_{i=1}^{N} \sum_{j=i+1}^{N} \log |x_i - x_j|.
\] (4.1)

Various numerical methods for global optimization are available (cf. [30], [21], [35]), including methods for non-smooth optimization and optimization with constraints. For low-dimensional problems, exact methods are available, whereas for higher-dimensional problems one often must use heuristic strategies, including evolution algorithms and simulated annealing. The following methods were used to confirm our numerical optimization results for (2.51b):

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. [1]).

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. [28]).

3) Lipschitz-Continuous Global Optimizer (LGO). This is a commercial globally optimization software program available for a number of software and hardware platforms, based on a combination of several rigorous (theoretically convergent) global minimization strategies, as well as a number of local minimization strategies. For further details, see [30].

On a unit sphere, it is convenient to write the location $x_j$ of each trap in terms of spherical coordinates ($\theta_j$, $\phi_j$), where $\theta_j$ is the latitude and $\phi_j$ is the longitude. To eliminate the effect of the rotational symmetries of the sphere, we fix the first trap $x_1$ at the north pole, i.e. $(\theta_1, \phi_1) = (0, 0)$, and we let $\phi_2 = 0$ for the second trap centered at $x_2$. Then, for \textit{N} traps on the unit sphere, one has a global optimization problem of $2\textit{N} - 3$ parameters in the range $0 < \theta_j \leq \pi$ for $j = 2, \ldots, N$, and $0 \leq \phi_j < 2\pi$ for $j = 3, \ldots, N$. As an “initial guess” for the global optimization routines, we chose the remaining traps $x_2, \ldots, x_N$ to be equally spaced on the equator $\theta = \pi/2$.

For $3 \leq \textit{N} \leq 20$ traps, the ECAM and DSO methods, as outlined above and implemented in the open software library GANSO [14], were used to obtain the numerical results in Table 2 for the global minimum of the discrete energy (2.51b) and the two classic energies of (4.1). A good agreement between the ECAM and DSO methods for the minimum values of these three discrete energy functions, as well as the optimal trap locations, were used to validate the results. For the classic discrete energies in (4.1), our results compare favorably with the tabulated data of [18], [11], and [33] for the Coulomb energy, and with the results of [3] for the logarithmic energy. From Table 2,
An Asymptotic Analysis of the Mean First Passage Time for Narrow Escape Problems

Table 2. Numerically computed minimal values of the discrete energy $\mathcal{H}$ of (2.51) for $3 \leq N \leq 20$, together with the optimal Coulomb and logarithmic energies in (4.1) for $N$-trap arrangements on the unit sphere. The results were obtained using both the ECAM and DSO methods.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\mathcal{H}$ (2.51)</th>
<th>$\mathcal{H}_c$ (4.1)</th>
<th>$\mathcal{H}_l$ (4.1)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>ECAM (DSO)</td>
<td>ECAM (DSO) [Ref.[18],[33]]</td>
<td>ECAM (DSO) [Ref. [3]]</td>
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<tr>
<td>3</td>
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<td>1.732051 (1.732051) [-]</td>
<td>-1.647918 (-1.647918)</td>
</tr>
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<td>3.674234 (3.674234) [3.674234]</td>
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</tr>
<tr>
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<tr>
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<td>-54.011130 (-54.011130)</td>
</tr>
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</table>

It is interesting to observe that for these values of $N$, the minimal Coulomb and logarithmic energies are monotone functions of $N$, whereas the energy (2.51) has a local minimum for $N = 9$ traps.

By using numerical optimization LGO software, further data for the optimal values of $\mathcal{H}$ for larger values of $N$ were computed by Prof. Raymond Spiteri, and these are given in Table 3. The numerical results in this table are believed to be correct to the number of significant digits shown.

Figure 3. The average MFPT $\bar{v}$ in (2.51) with $D = 1$ and the principal eigenvalue $\lambda$ of (3.26) with $c = 2/\pi$ and $a = 1$ versus the percentage trap surface area fraction $100f$, where $f = N\varepsilon^2/4$, for the optimal arrangement of $N$ identical circular traps of a common radius $\varepsilon$ on the boundary of the unit sphere. Left figure: $\bar{v}$ versus $100f$ for $N = 1, 5, 10, 20, 30, 40, 50, 60$ (top to bottom curves). Right figure: $\lambda$ versus $f$ for $N = 1, 5, 10, 20, 30, 40, 50, 60$ (bottom to top curves).

For $N$ circular traps of a common radius $\varepsilon$ the average MFPT $\bar{v}$ is given in (2.51), and the corresponding principal eigenvalue $\lambda$ is obtained upon setting $a = 1$ and $c = 2/\pi$ in (3.26). We then use the results for the optimum value of
\[ \mathcal{H} \]

as given in Table 3 to show the significant effect on the optimal of \( \bar{v} \) and \( \lambda \) of the fragmentation of the trap set on the surface of the unit sphere. The percentage surface area fraction of traps is \( 100f \), where \( f = N \pi \varepsilon^2 / 4\pi = N \varepsilon^2 / 4 \).

In Fig. 3(a) we plot \( \bar{v} \) versus \( 100f \) for the optimal arrangement of \( N = 5, 10, 20, 30, 40, 50, 60 \) traps on the surface of the unit sphere. In this figure we also plot \( \bar{v} \) for a single large trap having the same trap surface area fraction. In Fig. 3(b) we plot the corresponding optimal value for the principal eigenvalue versus \( 100f \). For \( N \) not too large, we conclude that even when \( f \) is small the effect of fragmentation of the trap set is rather significant. The clustering of the curves in Fig. 3(a) when \( N \) becomes larger suggests that the effect of fragmentation decreases significantly when the traps are sufficiently dispersed over the surface of the sphere.

To further illustrate our asymptotic results, we take \( N = 11 \) locally circular traps of a common radius \( \varepsilon \) and in Fig. 4(a) we plot \( \bar{v} \) in (2.51) versus \( \varepsilon \) for three different point arrangements on the sphere, including the set of points that minimize \( \mathcal{H} \) in (2.51 b). For \( N = 11 \) and \( \varepsilon = 0.2 \) the traps occupy 11% of the surface area of the sphere. The optimal point arrangement on the sphere is depicted in Fig. 4(b). From Fig. 4(a) we observe that a randomly generated point arrangement gives a result for \( \bar{v} \) that is rather close to that for the optimal point arrangement. For \( \varepsilon = 0.1907 \), the eleven traps occupy about 10% of the surface area of the sphere, and the optimal \( \bar{v} \) is \( \bar{v} \approx 0.368 \). We remark that for a single large trap with a 10% surface area fraction its radius must be \( \varepsilon = 0.6325 \). For this value of \( \varepsilon \), (2.45) yields \( \bar{v} \approx 1.48 \), which is about three times larger than for the optimal point arrangement. This example shows clearly the significant effect on \( \bar{v} \) of trap fragmentation.

Next, we discuss the spatial configuration of the optimal arrangement of traps for the range \( 2 \leq N \leq 20 \). For \( N = 2, 3, 4 \), the optimal trap arrangements for the discrete energy (2.51 b) and the two classical energies of (4.1) must
Figure 4. Left figure: Plot of the average MFPT $\bar{\nu}$ in (2.51) versus $\varepsilon$ for $D = 1$, $N = 11$, and three different arrangements of points on the sphere. The heavy solid curve corresponds to the minimum point of $\mathcal{H}$ in (2.51b), the solid curve is for eleven points equidistantly spaced on the equator, and the dotted curve is for a randomly generated point arrangement. Right figure: the optimal arrangement of $N = 11$ points on the sphere that minimize $\mathcal{H}$ in (2.51b).

To be the same, since equidistant spherical arrangements are available. For $N = 2$, the traps occupy the two poles; for $N = 3$ they are located at the vertices of an inscribed equilateral triangle; and for $N = 4$ they are located at the vertices of an inscribed tetrahedron. Moreover, as shown in Table 4, our numerical results predict that the optimal trap locations for each of the three discrete energies also coincide for $N = 5, 6, 8, 9, 10, 12$.

The numerically computed minimal energy arrangements for $N = 4, 5, 6$ are shown in Fig. 5. For $N = 5$ and $N = 6$, two traps are located at the poles, while the other $N - 2$ traps are on the equator. For $N = 8, 9, 10, 12$, the minimal energy arrangements are irregular and are shown in Fig. 6. For $N = 10, 12$, the minimal energy arrangements have two “belts” of traps with common latitude $\theta$, with two traps located at the poles.

Figure 5. Minimal energy trap configurations for $N = 4, 5, 6$ traps, common for the three energies.

Next, we consider cases where the optimal trap arrangements for the three different discrete energies do not coincide. For $N = 7$, numerically computed optimal trap arrangements are shown in Fig. 7, with the optimal coordinates of the trap locations given in Table 5. These results show that the minimum energy trap arrangement is the same for the Coulomb and logarithmic energies in (4.1), and consists of traps at the two poles and on the equator. In contrast, the discrete energy $\mathcal{H}$ of (2.51b) has a rather different optimal trap arrangement.
### Table 4. Spherical coordinates (θ, φ) of the optimal locations of N = 3, 4, 5, 6, 8, 9, 10, and 12 traps. These arrangements simultaneously minimize the discrete energy (2.51 b) and the two classical discrete energies in (4.1).

<table>
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<td>1.571</td>
<td>3.142</td>
<td></td>
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<tr>
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<td>1.571</td>
<td>1.571</td>
<td>1.571</td>
<td>3.142</td>
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<tr>
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<td>1.251</td>
<td>1.399</td>
<td>1.399</td>
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<td>1.207</td>
<td>1.325</td>
<td>1.325</td>
<td>1.561</td>
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<td>2.415</td>
<td>2.415</td>
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<tr>
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<td>0.000</td>
<td>1.134</td>
<td>1.134</td>
<td>1.134</td>
<td>1.134</td>
<td>2.007</td>
<td>2.007</td>
<td>2.007</td>
<td>2.007</td>
<td>3.142</td>
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<tr>
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<td>1.071</td>
<td>1.071</td>
<td>1.071</td>
<td>2.035</td>
<td>2.035</td>
<td>2.035</td>
<td>2.035</td>
<td>3.142</td>
</tr>
</tbody>
</table>

For N = 11, the optimal trap arrangements shown in Fig. 8 are irregular and different for the three discrete energy functions. The coordinates of the optimal trap locations are given in Table 6.

As shown in Fig. 9, for N = 16 the optimal trap arrangement is the same for the discrete energy $\mathcal{H}$ of (2.51 b) and the logarithmic energy $\mathcal{H}_L$ of (4.1), but is different for the Coulomb energy $\mathcal{H}_C$ of (4.1). The coordinates of the optimal trap locations are given in Table 7.

Finally, as shown in Fig. 10, the minimal energy trap arrangements for N = 20 is rather different for the three discrete energy functions. The coordinates of the optimal trap arrangements are given in Table 8. Interestingly, for
An Asymptotic Analysis of the Mean First Passage Time for Narrow Escape Problems

Figure 7. Minimal energy configurations for $N = 7$ traps. Left: the energy $\mathcal{H}$ of (2.51 b). Right: the Coulomb and logarithmic energies of (4.1).

<table>
<thead>
<tr>
<th>Energy</th>
<th>Spherical Coordinates of Optimal Trap Locations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{H}$</td>
<td>$\theta$</td>
</tr>
<tr>
<td></td>
<td>$\phi$</td>
</tr>
<tr>
<td>$\mathcal{H}_C$</td>
<td>$\theta$</td>
</tr>
<tr>
<td></td>
<td>$\phi$</td>
</tr>
</tbody>
</table>

Table 5. Spherical coordinates ($\theta, \phi$) of the optimal locations of $N = 7$ traps for the minimum of the energy $\mathcal{H}$ of (2.51 b), and the common minimum energy trap arrangement of the Coulomb and logarithmic energies in (4.1).

Figure 8. Minimal energy trap configurations for $N = 11$ traps. Left: the energy $\mathcal{H}$ of (2.51 b). Middle: the Coulomb energy of (4.1). Right: the logarithmic energy of (4.1).

The logarithmic energy in (4.1), the numerically computed minimum energy is attained in a multi-belt configuration, symmetric with respect to the equatorial plane $\theta = \pi/2$, with traps at both poles. In contrast, the optimal arrangements are much less regular for the other two discrete energies.

Finally, we formally derive a scaling law as $N \to \infty$ for the discrete energy $\mathcal{H}(x_1, \ldots, x_N)$ in (2.51 b). We decompose $\mathcal{H}$ into the sum of three terms as

$$\mathcal{H}(x_1, \ldots, x_N) = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3,$$

(4.2 a)
<table>
<thead>
<tr>
<th>Energy</th>
<th>Spherical Coordinates of Optimal Trap Locations</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathcal{H} )</td>
<td>( \theta )</td>
</tr>
<tr>
<td>( \phi )</td>
<td>0.000</td>
</tr>
<tr>
<td>( \mathcal{H}_C )</td>
<td>( \theta )</td>
</tr>
<tr>
<td>( \phi )</td>
<td>0.000</td>
</tr>
<tr>
<td>( \mathcal{H}_L )</td>
<td>( \theta )</td>
</tr>
<tr>
<td>( \phi )</td>
<td>0.000</td>
</tr>
</tbody>
</table>

Table 6. Spherical coordinates \((\theta, \phi)\) of the optimal locations of \(N = 11\) traps for the minimum of the energy \(\mathcal{H}\) of \((2.51 \, b)\), and the Coulomb and logarithmic energies of \((4.1)\).

\[
\mathcal{H}_1 = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{|x_i - x_j|}, \quad \mathcal{H}_2 = -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \log |x_i - x_j|, \quad \mathcal{H}_3 = -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \log (2 + |x_i - x_j|) . \quad (4.2 \, b)
\]

We then derive an approximation to the optimal value of \(\mathcal{H}_j\) as \(N \to \infty\) for \(j = 1, 2, 3\) by using the mean-field approximation method of [15] and [3].

We first consider the Coulomb term \(\mathcal{H}_1\), as was discussed in [15]. Suppose that a charge is located at the north
An Asymptotic Analysis of the Mean First Passage Time for Narrow Escape Problems

<table>
<thead>
<tr>
<th>Energy</th>
<th>Spherical Coordinates of Optimal Trap Locations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{H}$</td>
<td>$\theta$ 0.000 0.855 0.919 0.919 0.950 1.083 1.563 1.563</td>
</tr>
<tr>
<td></td>
<td>$\phi$ 0.000 1.111 3.930 5.113 2.539 6.247 1.758 3.221</td>
</tr>
<tr>
<td>$\mathcal{H}_L$</td>
<td>$\theta$ 1.742 1.742 1.764 2.032 2.032 2.452 2.604 2.657</td>
</tr>
<tr>
<td></td>
<td>$\phi$ 0.852 5.358 4.392 0.000 2.500 3.589 1.380 5.249</td>
</tr>
<tr>
<td>$\mathcal{H}_C$</td>
<td>$\theta$ 1.764 1.763 1.911 1.911 1.911 2.605 2.605 2.605</td>
</tr>
<tr>
<td></td>
<td>$\phi$ 3.733 5.827 0.525 2.620 4.714 1.445 3.540 5.634</td>
</tr>
</tbody>
</table>

Table 7. Spherical coordinates $(\theta, \phi)$ of the optimal locations of $N = 16$ traps for the Coulomb energy of (4.1), and the common minimum energy trap arrangement for the discrete energy $\mathcal{H}$ of (2.51 b) and the logarithmic energy of (4.1).

<table>
<thead>
<tr>
<th>Energy</th>
<th>Spherical Coordinates of Optimal Trap Locations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{H}$</td>
<td>$\theta$ 0.000 0.811 0.811 0.825 0.825 0.999 1.144 1.497 1.497 1.645</td>
</tr>
<tr>
<td></td>
<td>$\phi$ 0.000 0.912 5.371 2.129 4.154 3.142 0.000 1.523 4.760 0.675</td>
</tr>
<tr>
<td>$\mathcal{H}_C$</td>
<td>$\theta$ 1.632 1.631 1.644 1.802 1.243 2.273 2.274 2.438 2.437 2.946</td>
</tr>
<tr>
<td></td>
<td>$\phi$ 2.324 3.959 5.608 3.141 0.000 1.269 5.015 2.431 3.853 0.002</td>
</tr>
<tr>
<td>$\mathcal{H}_L$</td>
<td>$\theta$ 1.571 1.634 1.634 2.095 2.094 2.202 2.202 2.436 2.436 2.967</td>
</tr>
<tr>
<td></td>
<td>$\phi$ 4.713 0.768 5.515 0.000 3.142 2.108 4.175 0.991 5.292 3.141</td>
</tr>
</tbody>
</table>

Table 8. Spherical coordinates $(\theta, \phi)$ of the optimal locations of $N = 20$ traps for the energy $\mathcal{H}$ of (2.51 b), and the Coulomb and logarithmic energies of (4.1).

pole. We write its interaction energy $E_{1i}$ with the $i$th other charge as

$$E_{1i}^{(1)} = \frac{1}{r_{1i}}, \quad r_{1i} = |x_1 - x_i| = \sqrt{2(1 - \cos \theta)},$$

where $\theta$ is the azimuthal angle of the particle located at $x_i$. For large $N$ we assume that the charges are distributed “homogeneously” on the sphere, and that there is no charge in the azimuthal neighborhood $0 \leq \theta < \theta_0$ of the north pole, where $\theta_0 \ll 1$. Therefore, for $\theta_0 \ll 1$, the number density of charges is given approximately by

$$P(\theta, \phi) = \begin{cases} \frac{\pi}{2} & \text{for } \theta_0 < \theta < \pi, \\ 0 & \text{for } 0 < \theta < \theta_0, \end{cases}$$

where $\theta_0$ is determined from the condition that $\int_0^{2\pi} \int_{\theta_0}^{\pi} P(\theta, \phi) \sin \theta d\theta d\phi = N - 1$, which yields $\cos \theta_0 = 1 - 2/N$. For $N \gg 1$, we use $\cos \theta_0 \approx 1 - \theta_0^2/2$, to obtain $\theta_0 \approx \sqrt{4/N}$, as was given in [3].
Next, the interaction energy of the north-pole charge with the remaining charges can be calculated analytically as

\[ \epsilon_1 = \int_0^{2\pi} \int_0^{\pi} P(\theta, \phi) E_{1i}^{(1)} \sin \theta \, d\theta \, d\phi, \tag{4.3} \]

which can be calculated analytically as \( \epsilon_1 = -N \sin \left( N^{-1/2} \right) - 1 \). From a Taylor series expansion, valid for large \( N \), we can approximate the total energy of the particle configuration as

\[ H_1 = \frac{1}{2} N \epsilon_1 \approx \frac{1}{2} N^2 - \frac{1}{2} N^{3/2} + \frac{1}{12} N^{1/2} - \frac{1}{240} N^{-1/2} + \frac{1}{10080} N^{-3/2} - \frac{1}{725760} N^{-5/2} + O(N^{-3}). \tag{4.4} \]

In a similar way, the interaction energy \( \epsilon_2 \) for \( H_2 \) is given by

\[ \epsilon_2 = \frac{N}{4\pi} \int_0^{2\pi} \int_0^{\pi} E_{12i}^{(2)} \sin \theta \, d\theta \, d\phi, \quad E_{12i}^{(2)} = -\frac{1}{2} \log r_{1i}, \quad r_{1i} = \sqrt{2(1-\cos \theta)}, \tag{4.5} \]

which can be evaluated explicitly to yield

\[ \epsilon_2 = -\log \left[ \sin \left( N^{-1/2} \right) \right] \left[ -\frac{N}{2} + \cos^2 \left( N^{-1/2} \right) \right] + (2 \log 2 - 1) \cos^2 \left( N^{-1/2} \right). \tag{4.6} \]

From a Taylor series expansion, valid for \( N \gg 1 \), the total energy \( H_2 = N \epsilon_2 / 2 \) is estimated as

\[ H_2 \approx \frac{N^2}{8} (1 - 2 \log 2) - \frac{1}{8} N \log N \left[ \frac{1}{8} N(1 - 2 \log 2) + \frac{1}{24} \log N - \frac{1}{12} \log 2 \right] + N^{-1} \left( \frac{1}{144} + \frac{1}{90} \log 2 \right) - \frac{1}{180} N^{-1} \log N \left[ \frac{7}{6480} - \frac{11260 \log 2}{480} \right] + \frac{1}{2520} N^{-2} \log N + O(N^{-3}). \tag{4.7} \]

The second logarithmic term \( H_3 \) in (4.2 b) can be estimated in a similar way. We define \( \epsilon_3 \) as

\[ \epsilon_3 = \frac{N}{4\pi} \int_0^{2\pi} \int_0^{\pi} E_{13i}^{(3)} \sin \theta \, d\theta \, d\phi, \quad E_{13i}^{(3)} = -\frac{1}{2} \log (2 + r_{1i}), \quad r_{1i} = \sqrt{2(1-\cos \theta)}. \tag{4.8} \]

We obtain analytically that

\[ \epsilon_3 = \frac{N}{4} \left[ 2 \sin \left( N^{-1/2} \right) - (2 \log 2 - 1) \cos^2 \left( N^{-1/2} \right) - 2 - 2 \cos^2 \left( N^{-1/2} \right) \log \left[ 1 + \sin \left( N^{-1/2} \right) \right] \right]. \tag{4.9} \]

For \( N \gg 1 \), the resulting total energy \( H_3 = N \epsilon_3 / 2 \) is estimated from a Taylor series expansion as

\[ H_3 \approx \frac{N^2}{8} (1 + 2 \log 2) + \frac{1}{4} \log 2 + \frac{1}{6} N^{-1/2} - \left( \frac{1}{16} + \frac{1}{12} \log 2 \right) - \frac{1}{20} N^{-1/2} + N^{-1} \left( \frac{1}{48} + \frac{1}{90} \log 2 \right) + \frac{23}{5040} N^{-3/2} - N^{-2} \left( \frac{1}{480} + \frac{1}{1260} \log 2 \right) - \frac{31}{90720} N^{-5/2} + O(N^{-3}). \tag{4.10} \]

In Fig. 11(a) we compare the the sum \( H = H_1 + H_2 + H_3 \), obtained by adding (4.4), (4.7), and (4.10) (and neglecting the unspecified \( O(N^{-3}) \) terms), with the numerically computed results for the optimal values of \( H \) as given in Table 3. As seen in Fig. 11(a), the agreement is relatively close.

The mean-field approximation completely disregards the spatial distribution of the optimal arrangement of particles on the sphere, and therefore yields an approximate result whose precise asymptotic validity as \( N \to \infty \) is very difficult to assess. The highest power of \( N \) obtained by this approximation is presumably theoretically correct in analogy with previous rigorous results for the classical Coulomb or logarithmic energies (see [25], [32], and [33]). However, the coefficients of the lower-order terms should depend on the optimal trap arrangement. Therefore, in terms of some unknown coefficients \( b_j \) for \( j = 1, \ldots, 6 \), we postulate that for \( N \gg 1 \) the energy \( H \) has the form

\[ H \approx \mathcal{F}(N) = \frac{N^2}{2} (1 - \log 2) + b_1 N^{3/2} + b_2 N \log N + b_3 N + b_4 N^{1/2} + b_5 \log N + b_6, \tag{4.11 a} \]
as suggested by the various terms in (4.4), (4.7), and (4.10). The resulting least squares fit of (4.11) to the data in Table 3 yields

\[ b_1 \approx -0.5668, \quad b_2 \approx 0.0628, \quad b_3 \approx -0.8420, \quad b_4 \approx 3.8894, \quad b_5 \approx -1.3512, \quad b_6 \approx -2.4523. \] (4.11 b)

In Fig. 11(b) we show the scatter plot of the absolute error between \( \mathcal{F}(N) \) and the data for \( \mathcal{H} \) of Table 3. This figure indicates that \( \mathcal{F}(N) \) provides a very good approximation to the numerically computed optimal values of \( \mathcal{H} \).

Finally, by using the scaling law \( \mathcal{H} \approx \frac{N^2}{2} (1 - \log 2) + b_1 N^{3/2} \) for large \( N \), we obtain the following rough estimate of the minimum value of the average MFPT \( \bar{v} \) in (2.51) for the case of \( N \gg 1 \) circular traps of a common radius \( \varepsilon \):

\[ \bar{v} \sim \frac{\Omega}{4\varepsilon DN} \left[ 1 - \frac{\varepsilon}{\pi} \log \frac{\varepsilon N}{\pi} \left( \frac{1}{5} + \frac{4b_1}{\sqrt{N}} \right) \right]. \] (4.12 a)

In terms of the trap surface area fraction \( f \), given by \( f = N\varepsilon^2/4 \), (4.12 a) can be written equivalently as

\[ \bar{v} \sim \frac{\Omega}{8D\sqrt{fN}} \left[ 1 - \frac{\sqrt{fN}}{\pi} \log \left( \frac{4f}{N} \right) + \frac{2\sqrt{fN}}{\pi} \left( \frac{1}{5} + \frac{4b_1}{\sqrt{N}} \right) \right]. \] (4.12 b)

The result (4.12 b) should provide a decent approximation to \( \bar{v} \) for the case \( f \to 0 \) with \( N \) large but fixed. Although it is tempting to take the dual limit \( N \to \infty \) with \( f \) small but fixed in (4.12 b), we emphasize that the derivation of (2.51) pertained strictly to the limit of small trap radius \( \varepsilon \to 0 \) with \( N \) fixed. Therefore, such an interchange in the limiting procedure is hardly justified. A precise discussion of whether our optimal average MFPT results have any relationship to corresponding results that can be obtained from the dilute trap volume fraction limit of homogenization theory is an interesting open question.

### 5 Conclusion

The method of matched asymptotic expansions was used to calculate a three-term asymptotic expansion for the MFPT for escape from the unit sphere when there are \( N \) locally circular traps of asymptotically small radii on the
boundary of the unit sphere. The third term in this expansion was shown to depend on the spatial configuration of the traps on the surface of the sphere. For $N$ not too large, it was shown that the fragmentation of the trap set has a strong influence on the average MFPT for a fixed small trap surface area fraction.

We suggest four key open problems. The first open problem is to give a rigorous justification of the three-term asymptotic result (2.44) derived here formally by the method of matched asymptotic expansions. The second open problem is to derive a result analogous to (2.44) for the average MFPT for an arbitrary bounded three-dimensional domain that has $N$ asymptotically small windows of radius $\mathcal{O}(\varepsilon)$ on its boundary. Only the third term in such an expansion should depend on the relative locations of the absorbing windows on the domain boundary. Such an analysis would require detailed knowledge of the regular part of the surface Neumann Green’s function for an arbitrary three-dimensional domain. A two-term expansion for this MFPT, which is independent of the window locations, is given in [43] for an arbitrary bounded three-dimensional domain. A third open problem is to explore whether there is any relationship between results that can be obtained from the dilute trap fraction limit of homogenization theory and the results obtained herein for the scaling law for the discrete energy function for large $N$. Finally, a fourth open problem is to calculate a high-order asymptotic expansion for the average MPFT for the case of interior traps of small radii within a three-dimensional domain. Some results in this direction are given in [5].

Acknowledgements

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Appendix A The Surface Neumann Green’s Function for a Sphere

Here we calculate the explicit solution to (2.2). Since the singular point is on the boundary of the sphere, then $G_s(x; x_j) \sim (2\pi)^{-1}/|x - x_j|$ as $x \to x_j \in \partial\Omega$. Our goal is to calculate $G_s(x; x_j)$ analytically and to determine higher order terms in the singular behavior as $x \to x_j$. To solve (2.2) analytically, we let $|x|^2 = r^2$ and decompose $G_s$ as

$$G_s = \frac{1}{6|\Omega|} \left(|x|^2 + 1\right) + \tilde{G}_s + C,$$

where $C$ is a constant chosen to ensure that $\int_{\Omega} G_s \,dx = 0$. Then, we obtain from (A.1) and (2.2) that $\tilde{G}_s$ satisfies

$$\Delta \tilde{G}_s = 0, \quad x \in \Omega; \quad \left.\partial_r \tilde{G}_s\right|_{r=1} = \delta(\cos \theta - \cos \theta_j)\delta(\phi - \phi_j) - \frac{1}{4\pi}.$$  \hspace{1cm} (A.2)

Next, the boundary condition in (A.2) is expressed in terms of Legendre polynomials. This is done as follows:

**Lemma A.1:** Let $\gamma$ denote the angle between $x$ and $x_j$ so that $\cos \gamma = x \cdot x_j$. Then, we have the identity

$$\left.\partial_r \tilde{G}_s\right|_{r=1} = \delta(\cos \theta - \cos \theta_j)\delta(\phi - \phi_j) - \frac{1}{4\pi}\sum_{m=1}^{\infty} (2m + 1) P_m(\cos \gamma).$$ \hspace{1cm} (A.3)

**Proof:** We recall the completeness formula for the spherical harmonics $Y_{mn}$ given by (cf. [22])

$$\sum_{m=0}^{\infty} \sum_{n=-m}^{m} Y_{mn}^*(\theta_j, \phi_j)Y_{mn}(\theta, \phi) = \delta(\phi - \phi_j)\delta(\cos \theta - \cos \theta_j),$$ \hspace{1cm} (A.4)
where * denotes complex conjugate. The well-known addition theorem for Legendre polynomials (cf. [22]) states that
\[
\frac{(2m+1)}{4} P_m(\cos \gamma) = \sum_{n=-m}^{m} Y^*_m(\theta, \phi) Y_m(\theta, \phi).
\] (A.5)

Upon summing equation (A.5) from \(m=0\) to \(\infty\), and using (A.4) and \(P_0(\cos \gamma) = 1\), we obtain (A.3).

The solution to \(\nabla \tilde{G}_s = 0\), which satisfies the boundary condition in (A.3), is simply
\[
\tilde{G}_s = \frac{1}{4\pi} \sum_{m=1}^{\infty} \frac{(2m+1)}{m} r^m P_m(\cos \gamma) = \frac{1}{2\pi} \sum_{m=1}^{\infty} r^m P_m(\cos \gamma) + \frac{1}{4\pi} \sum_{m=1}^{\infty} \frac{r^m}{m} P_m(\cos \gamma).
\] (A.6)

We now calculate the two terms in (A.6) separately.

The well-known generating function \((1 - 2xt + t^2)^{-1/2} = \sum_{m=0}^{\infty} P_m(x) t^n\) shows that the first term in (A.6) is
\[
\frac{1}{2\pi} \sum_{m=1}^{\infty} r^m P_m(\cos \gamma) = \frac{1}{2\pi} \sqrt{1 - 2r \cos \gamma} - \frac{1}{2\pi} = \frac{1}{2\pi |x-x|} - \frac{1}{2\pi}.
\] (A.7)

Next, we define \(I(r) = \sum_{m=1}^{\infty} \frac{r^m}{m} P_m(\cos \gamma)\). By differentiating \(I\), and then using the generating function, we get
\[
I'(r) = \frac{1}{r} \sum_{m=1}^{\infty} r^m P_m(\cos \gamma) = \frac{1}{r} \left[ \frac{1}{\sqrt{1 - 2r \cos \gamma + r^2}} - 1 \right].
\] (A.8)

Since \(I(0) = 0\), we can integrate the equation above and then use \(|x-x| = (1 + r^2 - 2r \cos \gamma)^{1/2}\) to obtain
\[
I(r) = \sum_{m=1}^{\infty} \frac{r^m}{m} P_m(\cos \gamma) = \int_{0}^{r} \left( \frac{1}{s} \sqrt{1 - 2s \cos \gamma + s^2} - \frac{1}{s} \right) ds = \log \left( \frac{2}{1 - r \cos \gamma + |x-x|} \right),
\] (A.9)

which determines the second term in (A.6). Then, substituting (A.9) and (A.7) into (A.6), and using (A.1), we can write \(G_s\) up to an arbitrary constant \(C\) as
\[
G_s(x; x_j) = \frac{1}{8\pi} \left( |x|^2 + 1 \right) + \frac{1}{2\pi |x-x|} + \frac{1}{4\pi} \log \left( \frac{2}{1 - r \cos \gamma + |x-x|} \right) + C.
\] (A.10)

Finally, we use the integral condition in (2.2), written as \(\int_{0}^{\pi} \int_{0}^{1} G_s r^2 \sin \gamma dr d\gamma d\phi = 0\), to determine \(C\). Here, without loss of generality, we have chosen \(x_j\) to be at the north pole so that \(\gamma = \theta\). By orthogonality of the \(P_m(z)\), it follows that \(\int_{0}^{\pi} P_m(\cos \gamma) \sin \gamma d\gamma d\phi = 2\delta_{m,0}\), where \(\delta_{m,0}\) is Kronecker’s symbol, \(\delta_{n,n} = 1\) and \(\delta_{m,n} = 0\) if \(m \neq n\).

Therefore, this identity together with (A.9) shows that the integral over the sphere of the logarithmic term in (A.10) vanishes identically. Next, from (A.7) and \(P_0(z) = 1\), we use the same identity to calculate
\[
\frac{1}{2\pi} \int_{0}^{2\pi} \frac{1}{|x-x|} dx = \frac{1}{2\pi} \sum_{m=0}^{\infty} \int_{0}^{2\pi} \int_{0}^{\pi} \int_{0}^{r^m P_m(\cos \gamma)} (\sin \gamma) r^2 d\gamma d\phi dr = \frac{2}{3}.
\] (A.11)

In this way, we obtain that
\[
\int_{\Omega} G_s dx = \int_{0}^{2\pi} \int_{0}^{\pi} \int_{0}^{r^1} G_s r^2 \sin \gamma d\gamma d\phi dr = \frac{1}{2} \int_{0}^{1} (r^2 + 1) r^2 dr + \frac{2}{3} + \frac{4\pi C}{3} = 0,
\]
which yields \(C = -7/(10\pi)\) and determines \(G_s\) explicitly in (A.10). This completes the proof of Lemma 2.1.

**Appendix B: The Inner Problem for \(w_s\)**

Here we first derive the PDE (2.13) for the second inner correction term \(w_s\). Under the mapping \(\eta = \varepsilon^{-1}(1 - r)\), \(s_1 = \varepsilon^{-1} \sin \theta_j(\phi - \phi_j)\), and \(s_2 = \varepsilon^{-1}(\theta - \theta_j)\), we show that the Poisson equation (2.1 a) in spherical coordinates for
$v(r, \phi, \theta)$ transforms for $\varepsilon \to 0$ to (2.13). Let $w(\eta, s_1, s_2) = v[r(\eta), \phi(s_1), \theta(s_2)]$. Then, we calculate

\[ v_{rr} + \frac{2}{r} v_r = \varepsilon^{-2} w_{\eta\eta} - 2\varepsilon^{-1} w_\eta + \mathcal{O}(1), \]

\[ r^{-2} \left( v_{\theta\theta} + v_\theta \cot \theta \right) = (1 - \varepsilon \eta)^{-2} \left( \varepsilon^{-2} w_{s_2s_2} + \varepsilon^{-1} \cot \theta_j w_{s_2} + \mathcal{O}(1) \right) = \varepsilon^{-2} w_{s_2s_2} + \varepsilon^{-1} \left( 2\eta w_{s_2s_2} + \cot \theta_j w_{s_2} + \mathcal{O}(1) \right), \]

\[ \frac{1}{r^2 \sin^2 \theta} v_{\phi\phi} = \frac{(1 - \varepsilon \eta)^{-2}}{[\sin(\theta_j + s_2 \eta)]^2} \varepsilon^{-2} \sin^2 \theta_j w_{s_1s_1} + \varepsilon^{-1} \left( \left[ \frac{2\eta w_{s_1s_1} - 2\eta \cot \theta_j w_{s_1s_1} + \mathcal{O}(1) \right] \right). \]

Therefore, upon adding the three expressions above, we get that $\Delta v = -D^{-1}$ in (2.1 a) becomes

\[ \Delta v = \varepsilon^{-2} \left( w_{\eta\eta} + w_{s_1s_1} + w_{s_2s_2} \right) + \varepsilon^{-1} \left[ 2\eta w_{s_1s_1} + \cot \theta_j (w_{s_2} - 2\eta w_{s_2s_2}) \right] + \mathcal{O}(1) = -\frac{1}{D}. \] (B.1)

If we then expand $w \sim \varepsilon^{-1} w_0 + \log \left( \frac{\hat{z}}{\eta} \right) w_1 + w_2 + \cdots$ as in (2.12), we readily obtain (2.13) for $w_2$ upon using the leading-order equation $w_{0\eta\eta} = -\left( w_{0s_1s_1} + w_{0s_2s_2} \right)$ to simplify the coefficient of $\eta$ in (B.1).

Next, we analyze the solution $w_2$ to (2.13), with the prescribed far-field behavior in (2.31), in terms of the solution decomposition given in (2.32). Our analysis shows how the solution to this problem generates a monopole term in its far-field expansion as written in (2.35), where the monopole coefficient $\kappa_j$ in (2.35) is as given in (2.36).

We analyze (2.33) for the term $w_2$, in the decomposition (2.32) of $w_2$. Although (2.33) is an inhomogeneous problem involving the solution $w_c$ of the electrified disk problem (2.15), its solution $w_2$ can be determined analytically.

**Lemma B.1:** The solution to (2.33) is given explicitly by

\[ w_{2c} = -\frac{\eta^2}{2} w_{\eta\eta} - \frac{\eta}{2} w_{\eta c} + \frac{1}{2} \int_0^\eta w_c(z, s_1, s_2) \, dz + \mathcal{K}(s_1, s_2) + \mathcal{w}_2. \] (B.2)

Here $\mathcal{K}(s_1, s_2)$ satisfies a Poisson’s equation with a compactly supported forcing function, formulated as

\[ \mathcal{K}_{s_1s_1} + \mathcal{K}_{s_2s_2} = q(s_1, s_2); \quad \mathcal{K}(s_1, s_2) = \frac{c_j}{2} \log \sigma + o(1), \quad \text{as} \quad \sigma = (s_1^2 + s_2^2)^{1/2} \to \infty, \] (B.3 a)

where $c_j$ is defined by $w_c \sim c_j / \rho$ as $\rho \to \infty$, while $q(s_1, s_2)$ is defined in terms of the surface charge density of the electrified disk problem (2.15) by

\[ q(s_1, s_2) \equiv -\frac{1}{2} w_{\eta\eta}|_{\eta=0} I_1, \quad I_1 = \left\{ \begin{array}{ll} 1, & (s_1, s_2) \in \Omega \\ 0, & (s_1, s_2) \notin \Omega \end{array} \right., \] (B.3 b)

where $\Omega \equiv \{(s_1, s_2) | s_1^2 + s_2^2 \leq a_j^2\}$. Moreover, in terms of $\mathcal{K}(s_1, s_2)$, the function $w_{2h}$ in (B.2) satisfies Laplace’s equation in a half-space with mixed Dirichlet-Neumann boundary conditions, formulated as

\[ w_{2h\eta\eta} + w_{2h_{s_1s_1}} + w_{2h_{s_2s_2}} = 0, \quad \eta \geq 0, \quad -\infty < s_1, s_2 < \infty, \] (B.4 a)

\[ \partial_\eta w_{2h} = 0, \quad \eta = 0, \quad (s_1, s_2) \notin \Omega; \quad w_{2h} = -\mathcal{K}(s_1, s_2), \quad \eta = 0, \quad (s_1, s_2) \in \Omega, \] (B.4 b)

\[ w_{2h} = \mathcal{O}(\rho^{-1}), \quad \text{as} \quad \rho = (\eta^2 + s_1^2 + s_2^2)^{1/2} \to \infty. \] (B.4 c)

The solution $w_{2c}$ in (B.2) has the far-field asymptotic behavior

\[ w_{2c} = \frac{c_j}{2} \log(\eta + \rho) - \frac{c_j}{2\rho^2} (\eta^2 + s_2^2)^{1/2} \frac{c_j \kappa_j}{\rho} + \mathcal{O}(\rho^{-2}), \quad \text{as} \quad \rho \to \infty. \] (B.5)

We remark that the $o(1)$ condition in (B.3 a) and the decay condition in (B.4 c) determine $\mathcal{K}(s_1, s_2)$ and $w_{2h}$ uniquely. In addition, it is readily observed that the problem for $\mathcal{K}$ has the correct strength for the logarithmic singularity at infinity. To see this, we let $s = (s_1, s_2)$ and solve (B.3) in terms of the free-space Green’s function as

\[ \mathcal{K}(s_1, s_2) = \frac{1}{2\pi} \int_{\Omega} \log |s - \sigma| q(\hat{s}) \, d\hat{s} \sim \left( \frac{1}{2\pi} \int_{\Omega} q(\hat{s}) \, d\hat{s} \right) \log \sigma - \frac{s \cdot \mathcal{e}_j}{2\pi |s|^2} + \mathcal{O}(|s|^{-2}), \quad \text{as} \quad \sigma = |s| \to \infty, \] (B.6)

where $\mathcal{e}_j \equiv \int_{\Omega} \hat{s}_j q(\hat{s}) \, d\hat{s}$. Therefore, $K \sim d_0 \log \sigma + o(1)$ as $\sigma \to \infty$, where $d_0 = -\left( 4\pi \right)^{-1} \int_{\Omega} w_{c\eta}|_{\eta=0} \, d\hat{s}$. To identify that
Then, using the equation

\[ w_{2p} = -\frac{\eta^2}{2} w_{\eta\eta} - \frac{\eta}{2} w_{\eta} + \frac{1}{2} \int_0^\eta w_c(z, s_1, s_2) dz + \mathcal{K}(s_1, s_2), \]  

(B.7)
satisfies (2.33a). Denoting \( \mathcal{L} v \equiv v_{\eta\eta} + \Delta_s v \), where \( \Delta_s v \equiv v_{s_1 s_1} + v_{s_2 s_2} \), we calculate

\[ w_{2p\eta\eta} = -\frac{\eta^2}{2} w_{\eta\eta\eta\eta} - \frac{5\eta}{2} w_{\eta\eta\eta} - \frac{3}{2} w_{\eta\eta}, \]  

(B.8a)

\[ \Delta_s w_{2p} = -\frac{\eta^2}{2} \partial_\eta (\Delta_s w_c) - \frac{\eta}{2} \Delta_s w_c + \frac{1}{2} \int_0^\eta \Delta_s w_c dz + \Delta_s \mathcal{K}. \]  

(B.8b)

Then, using the equation \( w_{\eta\eta} = -\Delta_s w_c \) satisfied by \( w_c \), (B.8b) becomes

\[ \Delta_s w_{2p} = \frac{\eta^2}{2} w_{\eta\eta\eta\eta} + \frac{\eta}{2} w_{\eta\eta\eta} - \frac{1}{2} \int_0^\eta w_{zzz} dz + \Delta_s \mathcal{K} = \frac{\eta^2}{2} w_{\eta\eta\eta\eta} + \frac{\eta}{2} w_{\eta\eta\eta} - \frac{1}{2} w_{\eta\eta} + \frac{1}{2} w_{\eta\eta}|_{\eta=0} + \Delta_s \mathcal{K}. \]  

(B.9)

Upon adding (B.8a) and (B.9), we calculate \( \mathcal{L} w_{2p} = w_{2p\eta\eta} + \Delta_s w_{2p} \) as

\[ \mathcal{L} w_{2p} = -2\eta w_{\eta\eta} - 2w_{\eta \eta} + \frac{1}{2} w_{\eta\eta}|_{\eta=0} + \Delta_s \mathcal{K}(s_1, s_2). \]  

(B.10)

Therefore, when \( \mathcal{K}(s_1, s_2) \) satisfies the Poisson equation (B.3), it follows that \( w_{2p} \) satisfies the PDE (2.33a).

Next, we note from (B.2) that on \( \eta = 0 \) the boundary conditions \( \partial_\eta w_{2c} = 0 \) for \( (s_1, s_2) \notin \Omega \) and \( w_{2c} = 0 \) for \( (s_1, s_2) \in \Omega \) are satisfied provided that \( w_{2h} \) satisfies the boundary conditions in (B.4b).

Next, we determine the asymptotic far-field behavior of \( w_{2c} \) as defined in (B.2). We use \( w_c \sim c_j \rho^{-1} \) as \( \rho \to \infty \) with \( \rho = (\eta^2 + \sigma^2)^{1/2} \) and \( \sigma = (s_1^2 + s_2^2)^{1/2} \) to calculate

\[ -\frac{1}{2} \frac{\eta^2}{2} w_{\eta\eta} - \frac{1}{2} \eta w_{\eta} \sim -\frac{c_j}{2} \frac{\eta \sigma^2}{(\eta^2 + \sigma^2)^{1/2}}, \]  

as \( \rho \to \infty \),

(B.11a)

\[ \frac{1}{2} \int_0^\eta w_c(z, s_1, s_2) dz \sim \frac{c_j}{2} \int_0^\eta \frac{1}{(z^2 + \sigma^2)^{1/2}} dz = \frac{c_j}{2} \left[ \log \left( \eta + \sqrt{\eta^2 + \sigma^2} \right) - \log \sigma \right], \]  

as \( \rho \to \infty \).  

(B.11b)

Therefore, \( w_{2c} \) in (B.2) has the far-field behavior

\[ w_{2c} \sim \frac{c_j}{2} \log \left( \eta + \sqrt{\eta^2 + \sigma^2} \right) - \frac{c_j}{2} \frac{\eta \sigma^2}{(\eta^2 + \sigma^2)^{3/2}} - \frac{c_j}{2} \log \sigma + \mathcal{K} + w_{2h}. \]  

(B.12)

We observe that the first two terms on the right-hand side of (B.12) agree exactly with those in (2.33c). In order that the remaining terms in the far-field behavior (B.12) cancel, as indicated by (2.33c), we require that \( \mathcal{K} \sim \frac{c_j}{2} \log \sigma + o(1) \) as \( \sigma \to \infty \), as written in (B.3a), and that \( w_{2h} \to 0 \) as \( \rho \to \infty \), as given in (B.4c).

The problem (B.4) for \( w_{2h} \) is a mixed Dirichlet-Neumann boundary value problem for the Laplacian with a spatially inhomogeneous Dirichlet condition imposed on the absorbing window. As such, it follows that \( w_{2h} = O(\rho^{-1}) \) as \( \rho \to \infty \). Moreover, since \( \mathcal{K} \) is proportional to \( c_j \), we can write the far-field behavior for \( w_{2h} \) as

\[ w_{2h} = -\frac{c_j \mathcal{K}_j}{\rho} + O(\rho^{-2}), \]  

(B.13) as \( \rho \to \infty \).
for some monopole coefficient $\kappa_j$ to be determined.

We remark that up to this stage of the analysis in this appendix we have not assumed that the absorbing window $\Omega$ is a circular disk of radius $a_j$. All that has been required so far is that $w_c$ satisfies $\mathcal{L}w_c = 0$ with boundary conditions $\partial_n w_c = 0$ on $\eta = 0$, $(s_1, s_2) \notin \Omega$ and $w_c = 1$ on $\eta = 0$, $(s_1, s_2) \in \Omega$ with $w_c \sim c_j/\rho$ as $\rho \to \infty$.

For the special case of a circular absorbing window of radius $a_j$, we can solve (B.3) analytically and then explicitly calculate the coefficient $\kappa_j$ of the monopole term in (B.13). For a circular disk, the function $q$ in (B.3) is simply

$$q(s_1, s_2) = \pi^{-1} \left[ a_j^2 - \sigma^2 \right]^{-1/2},$$

where $\sigma = \left( s_1^2 + s_2^2 \right)^{1/2}$ (see p. 38 of [12]). Therefore, from (B.3), $\mathcal{K} = \mathcal{K}(\sigma)$ is the solution of the radially symmetric problem

$$\sigma^{-1} (\sigma \mathcal{K}_\sigma)_{\sigma} = \left\{ \begin{array}{ll}
\pi^{-1} \left[ a_j^2 - \sigma^2 \right]^{-1/2}, & 0 \leq \sigma < a_j, \\
0, & \sigma \geq a_j,
\end{array} \right. \quad (B.14)$$

with $\mathcal{K}(\sigma) = a_j \pi^{-1} \log \sigma$ for $\sigma \geq a_j$. The solution to (B.14) for $\sigma \leq a_j$ with $\mathcal{K}(a_j) = a_j \pi^{-1} \log(a_j)$ is simply

$$\mathcal{K}(\sigma) = \frac{1}{\pi} \left[ a_j \log \left( a_j + \sqrt{a_j^2 - \sigma^2} \right) - \sqrt{a_j^2 - \sigma^2} \right], \quad 0 \leq \sigma \leq a_j. \quad (B.15)$$

For a circular disk, the coefficient $\kappa_j$ of the monopole term in (B.13) can be calculated by using the known far-field behavior of $w_{2h}$ given by (see [10] or section 1.4 of [12])

$$w_{2h} \sim -\frac{2}{\pi \rho} \int_0^{a_j} \frac{\mathcal{K}(\sigma) \sigma}{\sqrt{a_j^2 - \sigma^2}} d\sigma, \quad \rho \to \infty. \quad (B.16)$$

The integral in (B.16) can be calculated explicitly by using (B.15) for $\mathcal{K}(\sigma)$. This yields,

$$J = \int_0^{a_j} \frac{\mathcal{K}(\sigma) \sigma}{\sqrt{a_j^2 - \sigma^2}} d\sigma = \frac{a_j^2}{\pi} \left[ \int_0^1 \frac{x}{\sqrt{1-x^2}} \left( \log \left[ 1 + \sqrt{1-x^2} \right] - \sqrt{1-x^2} \right) dx + \log a_j \int_0^1 \frac{x}{\sqrt{1-x^2}} dx \right], \quad (B.17)$$

which evaluates to $J = a_j^2 \pi^{-1} \left[ 2 \log 2 - \frac{3}{2} + \log a_j \right]$. Since $c_j = 2a_j/\pi$, it follows from (B.13) and (B.16) that

$$w_{2h} \sim -\frac{c_j \kappa_j}{\rho}, \quad \rho \to \infty, \quad \kappa_j = \frac{c_j}{2} \left[ 2 \log 2 - \frac{3}{2} + \log a_j \right]. \quad (B.18)$$

This detailed analysis of the solution to the inner problem for $w_2$ completes the proof of Lemma B.1 and justifies the far-field result (2.37) with $\kappa_j$ as given in (2.36).

Finally, we remark that the solution $w_{20}$ to (2.34) is odd in $s_2$ and therefore cannot generate a monopole term at infinity. The explicit solution to (2.34) is given in terms of the solution $w_c$ of the electrified disk problem (2.15) as follows:

**Lemma B.2:** The solution to (2.34) is given explicitly by

$$w_{20} = \cot \theta_j \left( \frac{s_1^2}{2} w_{c s_2} - s_2 s_1 w_{c x_1} \right). \quad (B.19)$$

It is readily verified that (B.19) incorporates the inhomogeneous terms in (2.34 a), satisfies the boundary conditions in (2.34 b), and has far-field asymptotic behavior that agrees with that in (2.34 c). We leave the verification of these details to the reader.

**References**

An Asymptotic Analysis of the Mean First Passage Time for Narrow Escape Problems


