# Traps, Holes, and Spots: Analysis and Modeling of Localization Behavior for Some Partial Differential Equations

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# Outline of the Talk

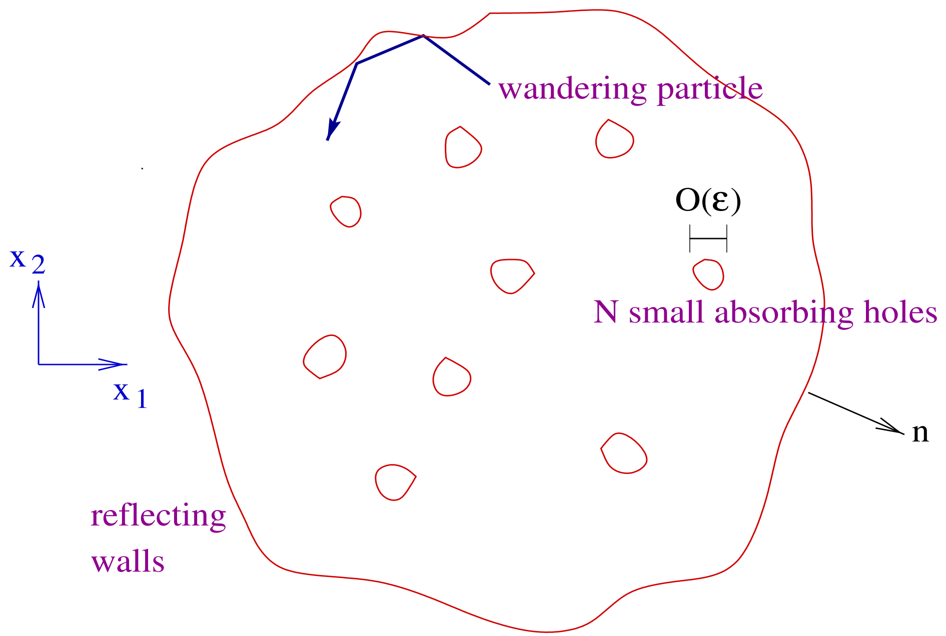
1. An Eigenvalue Optimization Problem in a Planar Domain
   - Asymptotic expansions, the Neumann Green's function, and Optimal Trap locations (Kolokolnikov, Titcombe, MJW).
   - Boundary Traps and a Narrow Escape Problem (Kolokolnikov, Pillay, MJW)
   - Analogous problems in a spherical domain (Cheviakov, Kolokolnikov, MJW)
2. Diffusion of Receptor Proteins on a Cylindrical Membrane
   - The reaction rate with one trap (Falcke, Straube, MJW)
   - Steady-state diffusion with many traps (Bressloff, Earnshaw, MJW)
3. Spot Solutions to Reaction-Diffusion Models
   - The stability of spots for the GM model (Kolokolnikov, MJW)
   - Self-Replication of spots for the Gray-Scott model (Chen, MJW). A self-destruction–self-replication "attractor"?
   - Self-Replication of spots for the Schnakenburg model on a growing domain (Kolokolnikov, MJW, Wei)

# Eigenvalue Problem with Interior Traps

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

$$\partial_n u = 0 \quad x \in \partial\Omega \,, \quad u = 0 \,, \quad x \in \partial\Omega_p \,.$$

- Here $\Omega_p = \cup_{i=1}^{N} \Omega_{\varepsilon_i}$ are $N$ interior non-overlapping holes or traps, each of 'radius' $O(\varepsilon) \ll 1$. The holes are assumed to be identical up to a translation and rotation.
- Also $\Omega_{\varepsilon_i} \to x_i$ as $\varepsilon \to 0$, for $i = 1, \ldots, N$. The centers $x_i$ are arbitrary.



# The Eigenvalue Optimization Problem

Goal: Let $\lambda_0 > 0$ be the fundamental eigenvalue. For $\varepsilon \to 0$ (small hole radius) find the hole locations $x_i$, for $i = 1, \ldots, N$, that maximize $\lambda_0$. In other words, chose the trap locations to minimize the lifetime of a wandering particle in the domain, i.e. where are the best places to fish?

**Specific Questions:**

- For $N = 1$ (one hole), is there a unique $x_0$ that maximizes $\lambda_0$? Can one find domains $\Omega$ where there are several values of $x_0$ that locally maximize $\lambda_0$?
- For the unit ball $\Omega = |x| \leq 1$, determine ring-type configurations of holes $x_1, ..., x_N$ that maximize $\lambda_0$.

Reference: T. Kolokolnikov, M. Titcombe, MJW, Optimizing the Fundamental Neumann Eigenvalue for the Laplacian in a Domain with Small Traps, EJAM Vol. 16, No. 2, (2005), pp. 161-200.

# Previous Studies I

For the Neumann problem, with $N$ circular holes each of radius $\varepsilon \ll 1$, Ozawa (Duke J. 1981) proved that

$$\lambda_0 \sim \frac{2\pi N \nu}{|\Omega|} + O(\nu^2), \qquad \nu \equiv \frac{-1}{\log \varepsilon} \ll 1 \,.$$

Since this is independent of $x_i$, $i = 1, \ldots, N$, we need the neglected $O(\nu^2)$ term to optimize $\lambda_0$. For the Dirichlet problem, Ozawa (1981) proved

$$\lambda_0 \sim \lambda_{0d} + 2\pi \sum_{i}^{N} \left[ u_0(x_i) \right]^2 \nu + O(\nu^2) \,.$$

To optimize $\lambda_0$, put the hole at a local maxima of $u_0$ (Harrell, (SIMA 2001)). For the Neumann or Dirichlet case, MJW, Henshaw, Keller (SIAP, 1993) showed

$$\lambda_0 \sim \lambda_*(\nu; x_1, ..x_N) + O(\varepsilon/\nu) \,,$$

where $\lambda_*$ (which "sums" all the log terms) satisfies a PDE that must be solved numerically. Highly accurate results for $\lambda_0$, but no analytical insight on how to optimize $\lambda_0$ wrt hole locations.

# Eigenvalue Asymptotics I

A singular perturbation analysis shows that all of the logarithmic terms are contained in the solution to

$$\Delta u^* + \lambda^* u^* = 0\,, \quad x \in \Omega \backslash \{x_1, \ldots, x_N\}\,,$$

$$\int_\Omega (u^*)^2 dx = 1\,; \qquad \partial_n u^* = 0\,, \quad x \in \partial\Omega\,,$$

$$u^* \sim A_j \, \nu_j \, \log|x - x_j| + A_j\,, \quad x \to x_j\,, \; j = 1, \ldots, N\,.$$

Here $\nu_j \equiv -1/\log(\varepsilon d_j)$, where $d_j$ is the logarithmic capacitance of the $j^{\text{th}}$ hole defined by

$$\Delta_y v = 0\,, \quad y \notin \Omega_j \equiv \varepsilon^{-1} \Omega_{\varepsilon_j}\,,$$

$$v = 0\,, \quad y \in \partial\Omega_j\,,$$

$$v \sim \log|y| - \log d_j + o(1)\,, \quad |y| \to \infty\,.$$

The highlighted term together with the normalization condition provides $N+1$ constraints for the $N+1$ unknowns $\lambda^*$ and $A_j$, for $j = 1, \ldots, N$.

# Eigenvalue Asymptotics II

Define the G-function $G(x, x_0, \lambda^*)$ for the Helmholtz operator as

$$\Delta G + \lambda^* G = -\delta(x - x_0)\,, \quad x \in \Omega\,; \quad \partial_n G = 0\,, \quad x \in \partial\Omega\,,$$

$$G(x;\,, x_0, \lambda^*) = -\frac{1}{2\pi} \log|x - x_0| + R(x; x_0, \lambda^*)\,.$$

Here $R$ is its "regular part". Then, $u^* = -2\pi \sum_{k=1}^{N} A_k \nu_k G(x; x_k, \lambda^*)$. Satisfying the point constraint at each $x_j$ gives the homogeneous system

$$A_j\left(1 + 2\pi\nu_j R(x_j; x_j, \lambda^*)\right) + 2\pi \sum_{\substack{k=1 \\ k\neq j}}^{N} A_k \nu_k G(x_j; x_k, \lambda^*) = 0\,, \quad j = 1, \ldots, N\,.$$

Consider the first eigenvalue for which $\lambda^* \to 0$ as $\varepsilon \to 0$. Set the determinant to zero and then use for $\lambda^* \ll 1$ that

$$G(x; x_0, \lambda^*) \sim -\frac{1}{|\Omega|\lambda^*} + G_m(x; x_0)\,, \quad R(x; x_0, \lambda^*) \sim -\frac{1}{|\Omega|\lambda^*} + R_m(x; x_0)\,,$$

where $G_m$ and $R_m$ are the Neumann G-function and its regular part.

# Eigenvalue Expansion: A Two-Term Result

**Principal Result:** For $N$ small circular holes centered at $x_1, \ldots, x_N$ with logarithmic capacitances $d_1, \ldots, d_N$, then

$$\lambda_0(\varepsilon) \sim \lambda^* , \quad \lambda^* = \frac{2\pi}{|\Omega|} \sum_{j=1}^{N} \nu_j - \frac{4\pi^2}{|\Omega|} \sum_{j=1}^{N} \sum_{k=1}^{N} \nu_j \nu_k \left(\mathcal{G}\right)_{jk} + O(\nu^3) \, .$$

Here $\nu_j \equiv= -1/\log(\varepsilon d_j)$ and $\left(\mathcal{G}\right)_{jk}$ are the entries of a certain Neumann Green's function matrix $\mathcal{G}$.

For $N$-circular holes each of radius $\varepsilon$ (for which $d_j = 1$), then with $\nu = -1/\log(\varepsilon)$,

$$\lambda_0(\varepsilon) \sim \lambda^* , \quad \lambda^* = \frac{2\pi N \nu}{|\Omega|} - \frac{4\pi^2 \nu^2}{|\Omega|} p(x_1, \ldots, x_N) + O(\nu^3) \, ,$$

where

$$p(x_1, \ldots, x_N) \equiv \sum_{j=1}^{N} \sum_{k=1}^{N} \left(\mathcal{G}\right)_{jk} \, .$$

Therefore, for $N$ circular holes and $\nu \ll 1$, $\lambda_0$ has a local maximum at a local minimum point of the “Energy-like” function $p(x_1, \ldots, x_N)$.

# The Neumann Green's Function

The Neumann Green's function $G_m(x; x_0)$, with regular part $R_m(x; x_0)$, satisfies:

$$\Delta G_m = \frac{1}{|\Omega|} - \delta(x - x_0)\,, \quad x \in \Omega\,,$$

$$\partial_n G_m = 0\,, \quad x \in \partial\Omega\,; \quad \int_\Omega G_m\, dx = 0\,,$$

$$G_m(x, x_0) = -\frac{1}{2\pi} \log|x - x_0| + R_m(x, x_0)\,;$$

The Green's matrix $\mathcal{G}$ is determined in terms of the hole-interaction term $G_m(x_i; x_j) \equiv G_{mij}$, and the self-interaction $R_m(x_i; x_i) \equiv R_{mii}$ by

$$\mathcal{G} \equiv \begin{pmatrix} R_{m11} & G_{m12} & \cdots & \cdots & G_{m1N} \\ G_{m21} & R_{m22} & G_{m23} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ G_{mN1} & \cdots & \cdots & G_{mNN-1} & R_{mNN} \end{pmatrix}.$$

# One Hole: Uniqueness of Maximizer?

**Corollary:** For the case of one circular hole of radius $\varepsilon$, centered at $x_1$, then

$$\lambda_0(\varepsilon) \sim \frac{2\pi\nu}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|} R_m(x_1; x_1) + O(\nu^3), \quad \nu \equiv -1/\log\varepsilon\,.$$

Thus $\lambda_0$ is maximized for a hole location that minimizes $R_m(x_1; x_1)$.

Is there a unique point $x_1$ in $\Omega$ that minimizes $R_m(x_1; x_1)$, and consequently maximizes $\lambda_0$?

- Require properties of $R_m(x; x_1)$ and $\nabla R_{m0} \equiv \nabla R_m(x : x_1)|_{x=x_1}$ (complex analysis).
- In a symmetric dumbbell-shape domain $x_1$ is unique. However, multiple roots of $\nabla R_m = 0$ can occur in non-symmetric dumbbell-shape domains (proof by complex analysis).

# Multiple Holes in the Unit Disk

Let $\Omega$ be the unit circle, so that $|\Omega| = \pi$. Then, $G_m$ and $R_m$ are

$$G_m(x;\xi) = -\frac{1}{2\pi}\log|x-\xi| + R_m(x;\xi)$$

$$R_m(x;\xi) = -\frac{1}{2\pi}\log\left|x|\xi| - \frac{\xi}{|\xi|}\right| + \frac{(|x|^2+|\xi|^2)}{2} - \frac{3}{4}\,.$$

For the unit disk, the problem of minimizing $p(x_1,\ldots,x_N)$ is equivalent to the problem of minimizing the function $\mathcal{F}(x_1,\ldots,x_N)$ defined by

$$\mathcal{F}(x_1,\ldots,x_N) = -\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N}\log|x_j-x_k| - \sum_{j=1}^{N}\sum_{k=1}^{N}\log|1-x_j\bar{x}_k| + N\sum_{j=1}^{N}|x_j|^2\,,$$

for $|x_j|<1$ and $x_j \neq x_k$ when $j \neq k$.

We consider the restricted optimization problem where $\mathcal{F}$ is optimized over certain ring-type configurations of holes. We then compare the results with those computed with optimization software from MATLAB.

# A Related Concentration Problem: Unit Disk

Our eigenvalue optimization problem is equivalent to minimizing

$$\mathcal{F}(x_1,\dots,x_N) = -\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N} \log|x_j - x_k| - \sum_{j=1}^{N}\sum_{k=1}^{N} \log|1 - x_j\bar{x}_k| + N\sum_{j=1}^{N}|x_j|^2\,,$$

for $|x_j| < 1$, and $x_j \neq x_k$ when $j \neq k$.

In contrast, by taking a certain limit of a variational formulation of the GL model of superconductivity in the unit disk, Lefter, Radulescu (1996) and Sandier, Soret (2000) showed that equilibrium vortices at $x_1,\dots,x_N$ inside the unit disk $|x_j| < 1$ with a common winding number are located at a minimum point of the renormalized energy $\mathcal{W}$ defined by

$$\mathcal{W}(x_1,\dots,x_N) = -\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N} \log|x_j - x_k| - \sum_{j=1}^{N}\sum_{k=1}^{N} \log|1 - x_j\bar{x}_k|\,.$$

This problem differs from that of the eigenvalue problem only by the confinement potential $N\sum_{j=1}^{N}|x_j|^2$.

# One-Ring Configurations: Unit Disk

Two Patterns: I (one ring), II (ring with a center hole). Specifically,

$$x_j = re^{2\pi ij/N}\,, \quad j = 1, \ldots, N\,, \quad \text{(P I)}\,,$$

$$x_j = re^{2\pi ij/(N-1)}\,, \quad j = 1, \ldots, N-1\,,\ x_N = 0\,, \quad \text{(P II)}\,.$$

More generally, we can construct $m$ ring patterns with $m$ rings of radii $r_1, \ldots, r_m$, with $r_j < r_{j+1}$, inside the unit disk. Assume that there are $J_k$ holes on the ring of radius $r_k$. On the $k^{\text{th}}$ ring, for $k = 1, \ldots, m$, the centres of the holes are assumed to satisfy

$$\xi_j^{(k)} = r_k e^{2\pi ij/J_k} e^{i\phi_k}\,, \quad j = 1, \ldots, J_k\,.$$

Here $\phi_k$ is a phase angle with $\phi_1 = 0$.

For each pattern we can calculate $p(x_1, \ldots, x_N)$ explicitly and then optimize over the ring radii.

# Pattern I

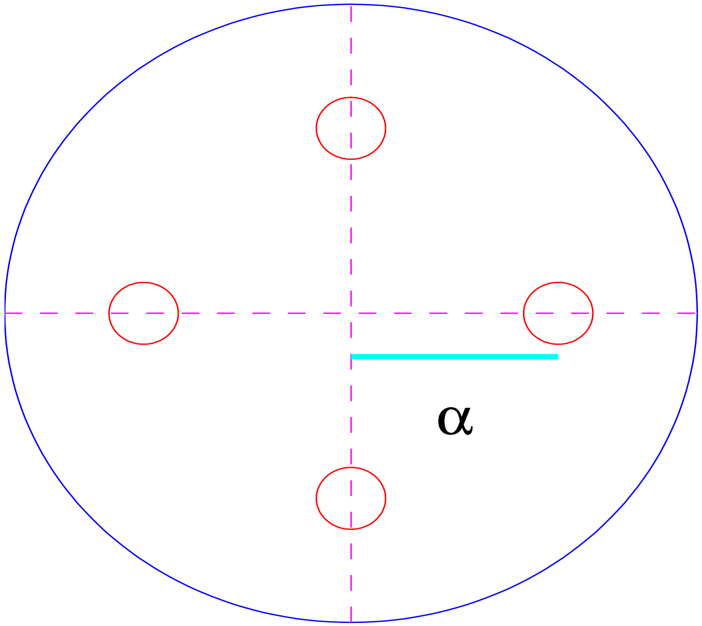
**Principal Result: (Pattern I):** Let $N > 1$, then $p = p_*/(2\pi)$ satisfies

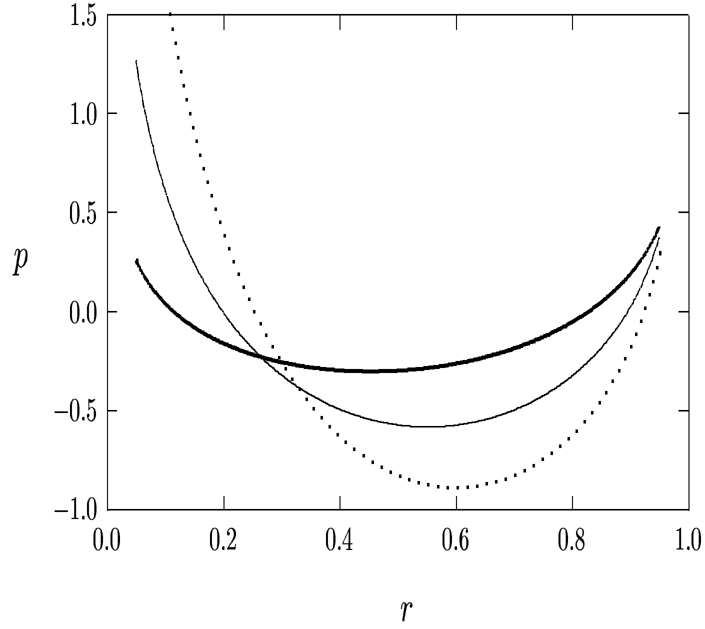
$$p_* = -N\log(Nr^{N-1}) - N\log\left(1 - r^{2N}\right) + r^2N^2 - \frac{3N^2}{4}\,.$$

Hence $p(r)$ has a unique minimum at $r = r_c$, where

$$\frac{r^{2N}}{1 - r^{2N}} = \frac{N-1}{2N} - r^2\,.$$

Left: $4$ holes on a ring. Right: $p$ versus $r$ for $N = 2, 3, 4$ holes on a ring.



# Pattern II

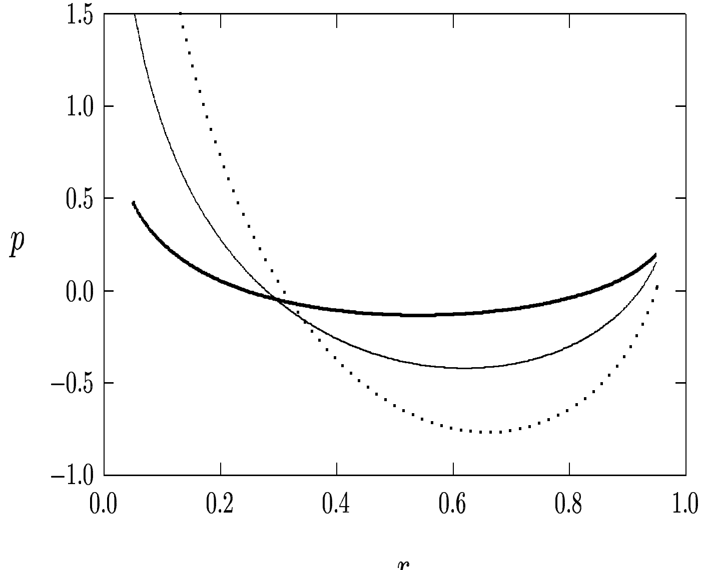
**Principal Result: (Pattern II):** Let $N > 1$, then $p = p_*(r)/(2\pi)$ satisfies

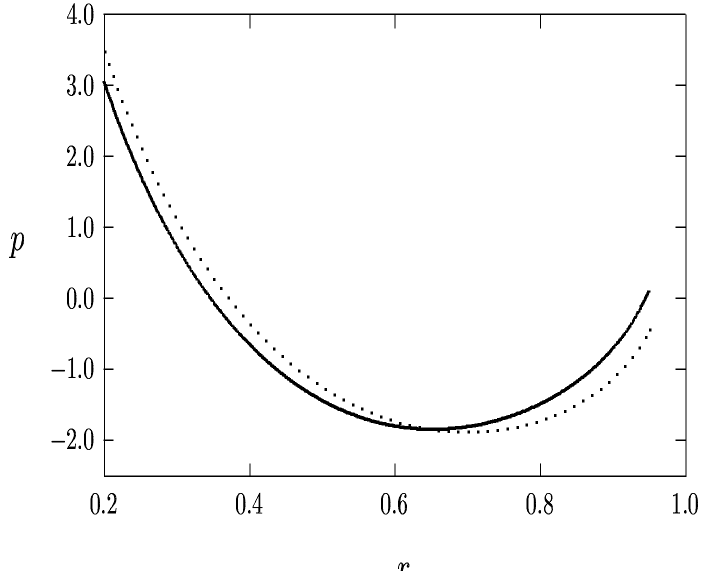
$$p_* = -(N-1)\log\left[(N-1)r^N\right] + r^2 N(N-1) - \frac{3N^2}{4} - (N-1)\log\left(1 - r^{2(N-1)}\right) \,.$$

Hence $p(r)$ has a unique minimum at $r = r_c$, where

$$\frac{r^{2N-2}}{1 - r^{2N-2}} = \frac{N}{N-1}\left(\frac{1}{2} - r^2\right) \,.$$

Left: $N = 2, 3, 4$ holes on a ring and a center hole. Right: $7$ holes on a ring (heavy solid) and $6$ holes on a ring with an extra center hole (dotted).



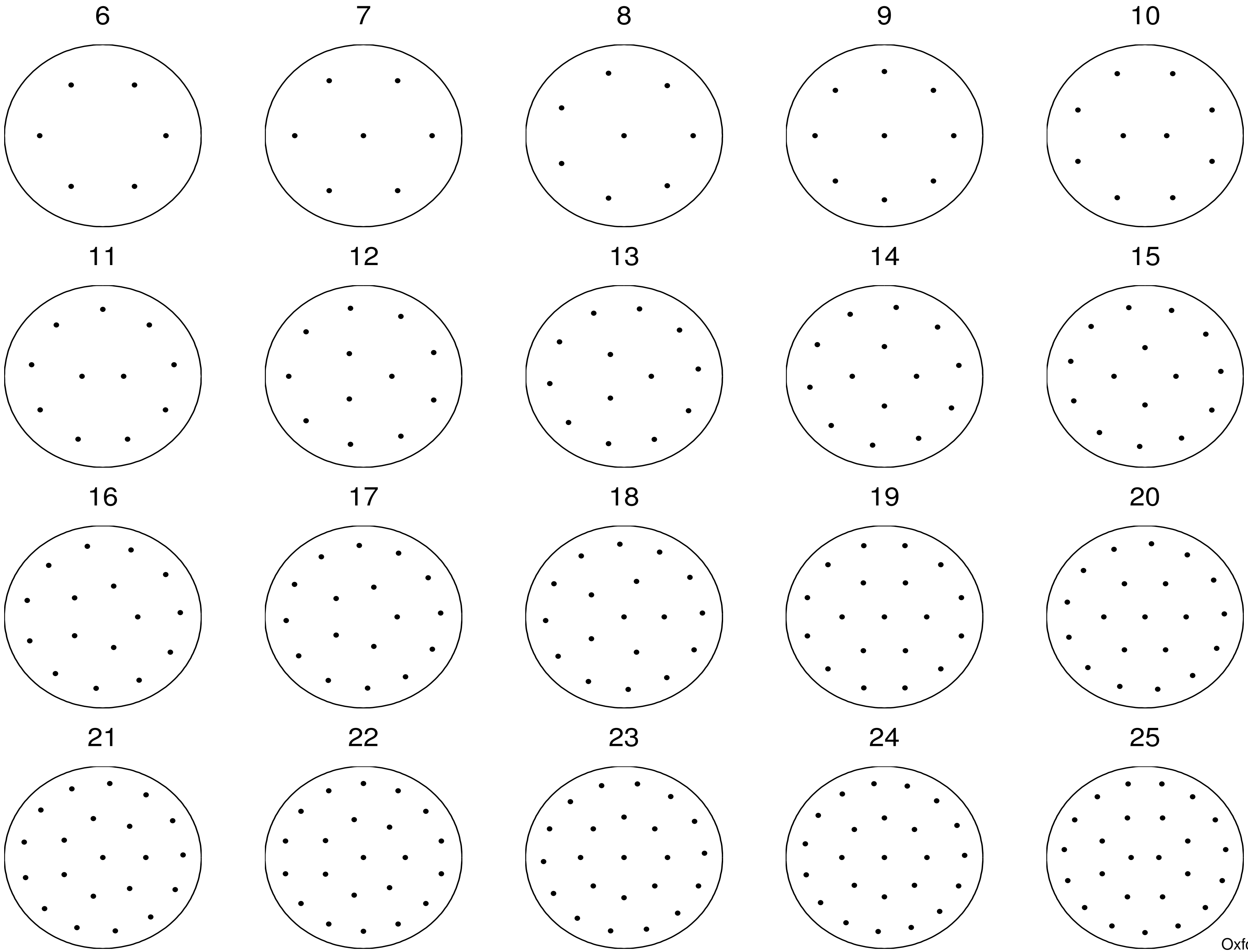



# Restricted Optimization: $m$-ring Patterns

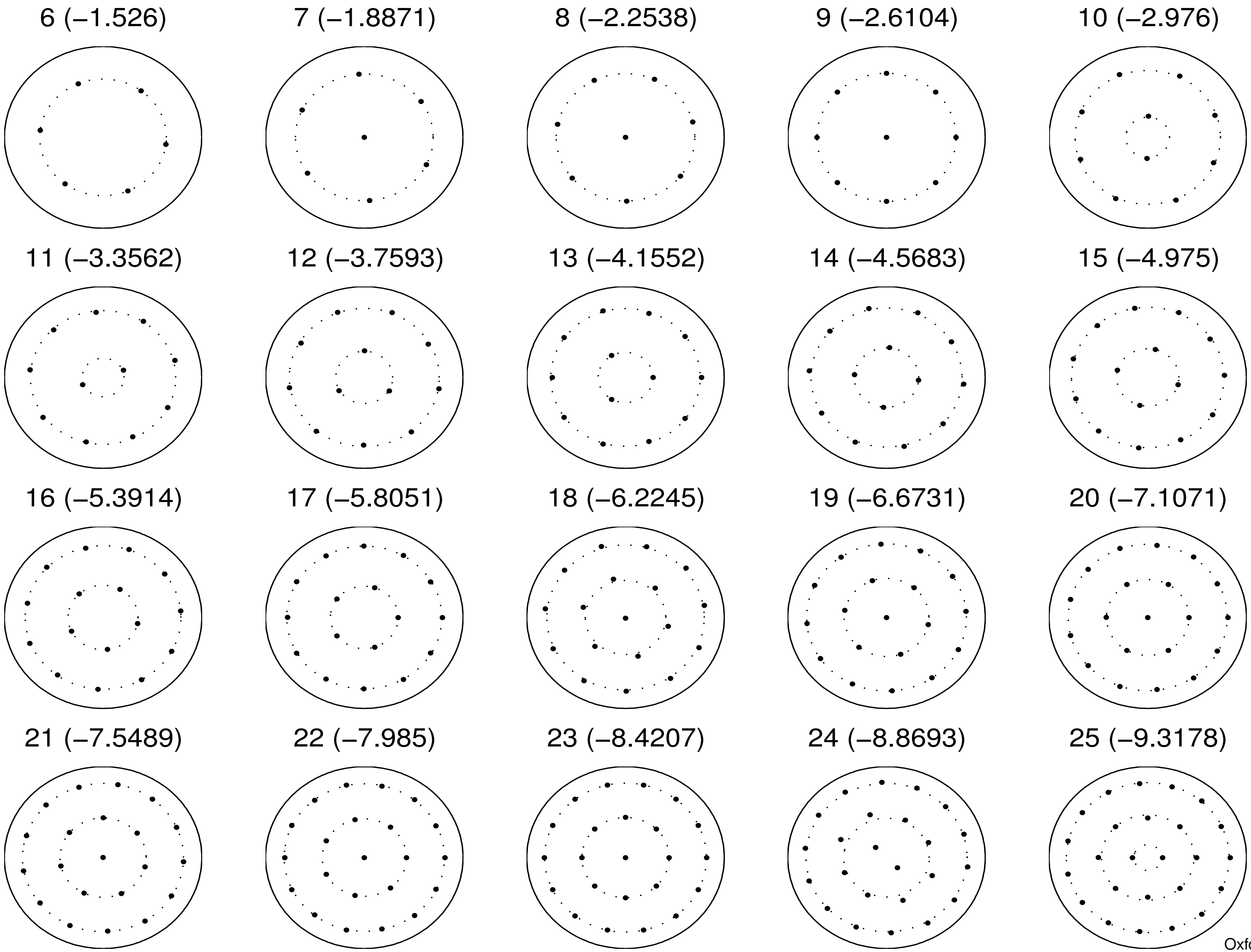
| $N$ | optimal pattern | $p_{\min}$ | optimum $r_j$ | second best pattern | $p$ |
|---|---|---|---|---|---|
| 6 | (6) | -1.5260 | 0.642 | [1](5) | -1.5134 |
| 7 | [1](6) | -1.8871 | 0.698 | (7) | -1.8398 |
| 8 | [1](7) | -2.2538 | 0.702 | (2,6) | -2.1732 |
| 9 | [1](8) | -2.6104 | 0.705 | (2,7) | -2.5754 |
| 10 | (2,8) | -2.9686 | 0.222, 0.737 | [1](9) | -2.9549 |
| 11 | (2,9) | -3.3498 | 0.212, 0.736 | (3,8) | -3.3449 |
| 12 | (3,9) | -3.7546 | 0.288, 0.760 | (2,10) | -3.7175 |
| 13 | (3,10) | -4.1511 | 0.277, 0.758 | (4,9) | -4.1457 |
| 14 | (4,10) | -4.5660 | 0.327, 0.776 | (3,11) | -4.5336 |
| 15 | (4,11) | -4.9728 | 0.316, 0.773 | (5,10) | -4.9636 |
| 16 | (5,11) | -5.3903 | 0.354, 0.788 | (4,12) | -5.3652 |
| 17 | (5,12) | -5.8040 | 0.343, 0.785 | [1](5,11) | -5.7921 |
| 18 | [1](5,12) | -6.2242 | 0.408, 0.797 | (6,12) | -6.2195 |
| 19 | [1](6,12) | -6.6713 | 0.429, 0.809 | [1](5,13) | -6.6422 |
| 20 | [1](6,13) | -7.1052 | 0.418, 0.805 | [1](7,12) | -7.0983 |
| 21 | [1](7,13) | -7.5480 | 0.436, 0.815 | [1](6,14) | -7.5257 |
| 22 | [1](7,14) | -7.9844 | 0.426, 0.811 | [1](6,15) | -7.9313 |
| 23 | [1](8,14) | -8.4204 | 0.442, 0.819 | [1](7,15) | -8.4058 |
| 24 | [1](8,15) | -8.8566 | 0.433, 0.816 | (2,8,14) | -8.8561 |
| 25 | (2,8,15) | -9.3056 | 0.141, 0.469, 0.824 | (3,8,14) | -9.3020 |

Table 1: Numerical results for the optimum configuration within the class of two and three-ring patterns with or without a centre hole. The first three columns indicate the optimum configuration, the minimum value of $p$, and the optimum ring radii. The last two columns correspond to the second best pattern. The notation $[1](5, 12)$ indicates a two-ring pattern with a centre hole, which has 5 and 12 holes on the inner and outer rings, respectively.

# Restricted Optimization: $m$-ring Patterns II

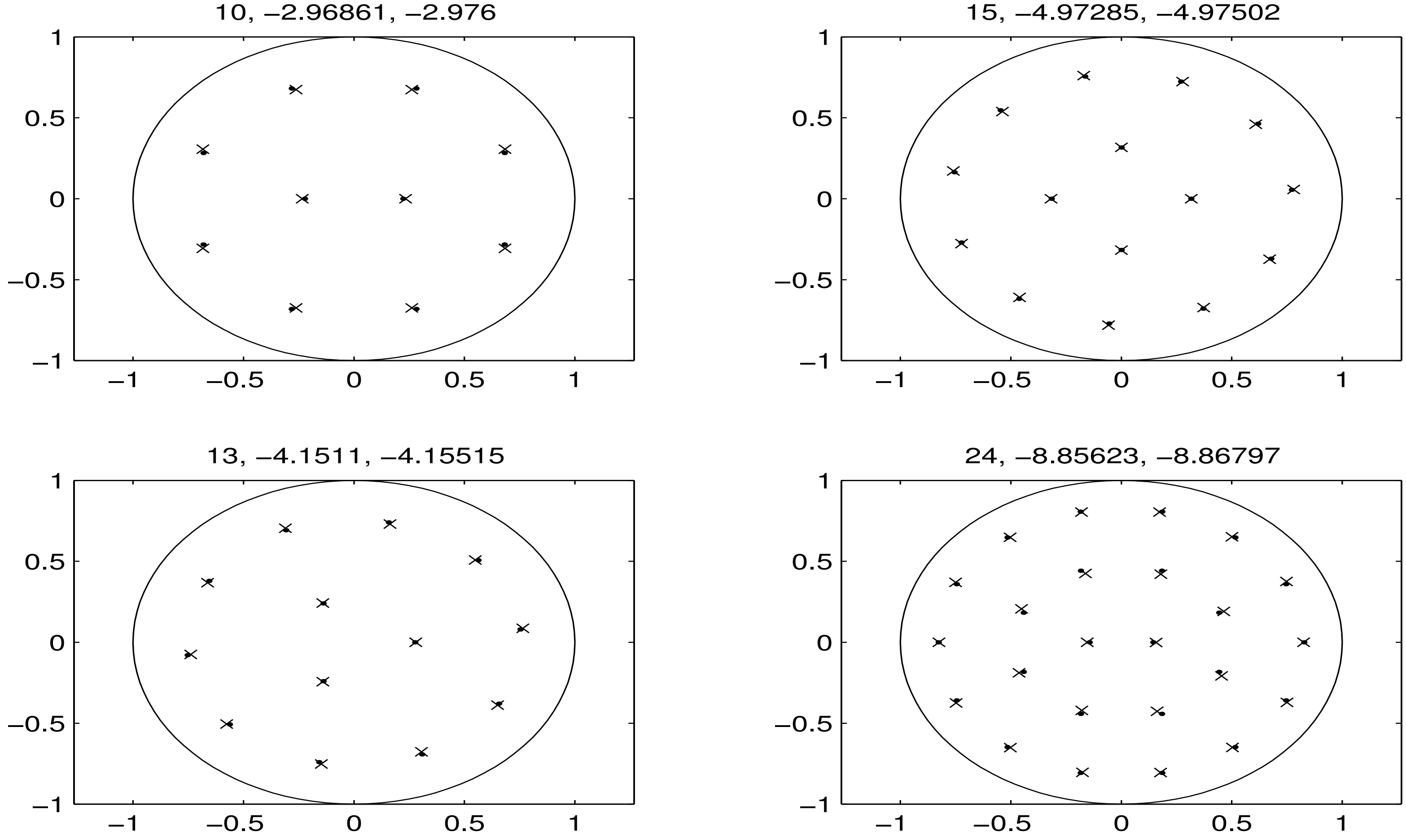


# Full Optimization: $m$-ring Patterns II



# Comparison: Restricted and Full Optimization

Optimization with respect to radii (dots) is compared with a MATLAB optimization with respect to $2N$ variables




Open: Is a Hexagonal Lattice the optimal arrangement for $N \gg 1$?

Open: Optimal Configurations in Other Domains such as a Square?

# Eigenvalue Problem with Boundary Traps: I

Consider the 2-D problem with boundary traps

$$\Delta u + \lambda u = 0 \,, \quad x \in \Omega \,; \quad \int_\Omega u^2 \, dx = 1 \,,$$

$$\partial_n u = 0 \quad x \in \partial\Omega_r \,, \quad u = 0 \,, \quad x \in \partial\Omega_a = \cup_{j=1}^{N} \partial\Omega_{\varepsilon_j} \,.$$

Assume that $\partial\Omega_{\varepsilon_j} \to x_j$ as $\varepsilon \to 0$ and $|\partial\Omega_{\varepsilon_j}| = 2\varepsilon$ for $j = 1, \ldots, N$. Then, with $\nu \equiv -1/\log[\varepsilon/2]$, the first eigenvalue $\lambda_1$ satisfies

$$\lambda_1 \sim \frac{\pi N \nu}{|\Omega|} - \frac{\pi^2 \nu^2}{|\Omega|} \sum_{j=1}^{N} \sum_{k=1}^{N} (\mathcal{G})_{jk} + O(\nu^3) \,,$$

where $(\mathcal{G})_{jk} \equiv G_m(x_j; x_k)$ for $j \neq k$ and $(\mathcal{G})_{jj} \equiv R_m(x_j; x_j)$ where $G_m(x; x_0)$ and $R_m(x; x_0)$ are now the "surface" Neumann G-function:

$$\Delta G_m = \frac{1}{|\Omega|} \,, \quad x \in \Omega \,; \quad \int_\Omega G_m(x; x_0) \, dx = 0 \,,$$

$$\partial_n G_m = 0 \,, \;\; x \in \partial\Omega_r \backslash \{x_0\} \,; \quad G_m(x, x_0) = -\frac{1}{\pi} \log|x - x_0| + R_m(x, x_0) \,.$$

# Eigenvalue Problem with Boundary Traps: II

Some consequences and open issues:

- For one patch, $\lambda_1$ and the associated "outer" eigenfunction $u_1$ are

$$\lambda_1 \sim \frac{\pi\nu}{|\Omega|} - \frac{\pi^2\nu^2}{|\Omega|} R_m(x_1, x_1) + \cdots \,,$$

$$u_1 \sim |\Omega|^{-1/2} - \frac{\pi\nu}{|\Omega|^{1/2}} G_m(x; x_1) + O(\nu^2)\,.$$

  Open: Is the point that minimizes $R_m$, and consequently maximizes $\lambda_1$, related to extrema of the boundary curvature?

- For $N$ patches on the boundary of the unit disk, for which $R_m$ is independent of $x_j$, the optimal arrangement is to choose $x_j$ with $|x_j| = 1$ for $j = 1, \ldots, N$ such that $\mathcal{F}(x_1, \ldots, x_N)$ is minimized, where

$$\mathcal{F}(x_1, \ldots, x_N) = -\sum_{j=1}^{N} \sum_{\substack{k=1 \\ k\neq j}}^{N} \log |x_j - x_k|\,.$$

  Clearly, we must choose the roots of unity. Open: what about the optimal arrangement for a general boundary?

# Narrow Escape: A Boundary Trap in 2-D

Consider Brownian motion with diffusivity $D$ in a 2-D domain $\Omega$ with a boundary that is insulated except for a small absorbing patch $\partial\Omega_a$ with $|\partial\Omega_a| = 2\varepsilon$. Assume that $\partial\Omega_a \to x_1$ as $\varepsilon \to 0$ and that the initial point for the Brownian motion is $X(0) = x \in \Omega$.

Let $v(x)$ be the mean first passage time (MFPT)

$$v(x) = E\left[\tau | X(0) = x\right] .$$

It is well-known that $v(x)$ satisfies

$$\Delta v = -\frac{1}{D}, \quad x \in \Omega ,$$
$$\partial_n v = 0 \quad x \in \partial\Omega_r ; \quad v = 0 , \quad x \in \partial\Omega_a .$$

Goal: Calculate $v(x)$ as $\varepsilon \to 0$.

History: The paper [SSH]: "Narrow Escape Part II: The Circular Disk", A. Singer, Z. Schuss, D. Holcman, J. Stat. Phys. Vol. 122, (2006), pp. 465-489. Very complicated analysis based on dual integral equations, special functions etc.... (also Narrow Escape Part I: (the Sphere) J. Stat. Phys. (2006) 26 pages, Narrow Escape Part III: Non-Smooth Domains etc...).

# Narrow Escape: A Boundary Trap in 2-D

Alternative More General Derivation: Expand $v$ in terms of the eigenfunctions $u_i$ for $i \geq 1$. Then,

$$v = \frac{1}{D\lambda_1}\left(\int_\Omega u_1\, dx\right) u_1 + \sum_{i=2}^{\infty} \frac{1}{D\lambda_i}\left(\int_\Omega u_i\, dx\right) u_i\,,$$

$$v \sim \frac{1}{D\lambda_1}\left(\int_\Omega u_1\, dx\right) u_1 + O(\varepsilon)\,.$$

This follows since $\lambda_1 = O(\nu)$ and $\lambda_i = O(1)$ for $i \geq 2$, with $\int_\Omega u_i\, dx = O(\varepsilon)$ for $i \geq 2$ by the Divergence theorem.

Use the asymptotics for $\lambda_1$ and the "outer" form for $u_1$. In 3-lines we get

$$v(x) = E\left[\tau | X(0) = x\right] \sim \frac{|\Omega|}{\pi D}\left[-\log\varepsilon + \log 2 + \pi(R_m(x_1;x_1) - G_m(x;x_1)\right]\,,$$

where $R_m$ and $G_m$ are the surface Neumann G-functions.

For the unit disk, $R_m = (8\pi)^{-1}$ and $G_m$ is known/ For example, if $x_1 = 1$ and $x = 0$, then we readily recover a result of [SSH]:

$$v(0) = E\left[\tau | X(0) = 0\right] \sim \frac{|\Omega|}{\pi D}\left[-\log\varepsilon + \log 2 + \frac{1}{4}\right]\,.$$

# Eigenvalues in 3-D Domains: Interior Traps I

In a 3-D bounded domain $\Omega$ consider

$$\Delta u + \lambda u = 0 \,, \quad x \in \Omega \backslash \Omega_p \,; \quad \int_{\Omega \backslash \Omega_p} u^2 \, dx = 1 \,,$$
$$\partial_n u = 0 \quad x \in \partial \Omega \,, \quad u = 0 \,, \quad x \in \partial \Omega_p \,.$$

Here $\Omega_p = \cup_{i=1}^{N} \Omega_{\varepsilon_i}$, with $\Omega_{\varepsilon_i} \to x_i$ as $\varepsilon \to 0$ and non-overlapping.

The first eigenvalue has the asymptotics

$$\lambda_1 \sim \frac{4\pi\varepsilon}{|\Omega|} \sum_{j=1}^{N} C_j - \frac{16\pi^2\varepsilon^2}{|\Omega|} \sum_{j=1}^{N} \sum_{k=1}^{N} C_j C_k \left(\mathcal{G}\right)_{jk} + O(\varepsilon^3) \,.$$

Here $\left(\mathcal{G}\right)_{jk} \equiv G_m(x_j; x_k)$ for $j \neq k$ and $\left(\mathcal{G}\right)_{jj} \equiv R_m(x_j; x_j)$ where $G_m(x;\xi)$ and $R_m(x;\xi)$ are now the 3-D Neumann G-function.

Also $C_j$ is the electrostatic capacitance of the $j^{\text{th}}$ hole defined by

$$\Delta v = 0 \,, \quad y \notin \Omega_j = \varepsilon^{-1} \Omega_{\varepsilon_j} \,,$$
$$v = 1 \,, \quad y \in \partial \Omega_j \,; \quad v \sim -\frac{C_j}{|y|} \,, \quad |y| \to \infty \,.$$

# Eigenvalues in 3-D Domains: Interior Traps II

The matrix $\mathcal{G}$ can be found explicitly when $\Omega$ is the unit sphere. By summing series related to Legendre polynomials

$$G_m(x;\xi) = \frac{1}{4\pi|x-\xi|} + \frac{1}{4\pi|x|r'} + \frac{1}{4\pi}\ln\left[\frac{2}{1-|x||\xi|\cos\theta + |x|r'}\right] + \frac{1}{8\pi}\left(|x|^2 + |\xi|^2\right) - \frac{13}{20\pi}\,.$$

Here $r' = |x' - \xi|$, where $x' = x/|x|^2$ is the image point and $\theta$ is the angle between $x$ and $\xi$. The regular part $R_m(\xi,\xi)$ is

$$R_m(\xi,\xi) = \frac{1}{4\pi\left(1-|\xi|^2\right)} - \frac{1}{4\pi}\log\left(1-|\xi|^2\right) + \frac{|\xi|^2}{4\pi} - \frac{13}{20\pi}\,.$$

Open: Where are the optimal trap locations $x_j$ for $j = 1, \ldots, N$ inside the unit sphere that maximize the first eigenvalue? For identical traps we need to minimize the explicitly known function $p(x_1, \ldots, x_N) = \sum\sum \mathcal{G}_{jk}$.

Open: What about more general domains such as $\Omega$ a cube. Here we need Ewald summation techniques to build the matrix $\mathcal{G}$.

# Eigenvalues in 3-D Domains: Boundary Traps

Consider a spherical domain $\Omega$ with $N$-small non-overlapping absorbing boundary patches on an otherwise reflecting boundary.

Open: Where are the optimal locations to put $N$ small patches to maximize the first eigenvalue $\lambda_1$?

One might guess that the trap locations that maximize $\lambda_1$ are given by the minimum of the discrete energy $\mathcal{F}(x_1, \ldots, x_N)$ defined by

$$\mathcal{F}(x_1, \ldots, x_N) = \sum_{j=1}^{N} \sum_{\substack{k=1 \\ k \neq j}}^{N} \frac{1}{|x_j - x_k|}, \qquad |x_j| = 1 .$$

If so, this is a famous discrete optimization problem of finding the minimal discrete energy of “electrons” confined to the boundary of a sphere. This is related to the discovery of Carbon-60 molecules. Long list of references; E. Saff, N. Sloane, A. Kuijlaars etc..

The difficulty with this problem is that the number of local minima grow exponentially with $N$, and so finding the global minimum is not trivial computationally.

# Biomembrane Surface Diffusion With Trap I

Consider the diffusion of proteins on the cylindrical surface (a biomembrane) of length $2L$ and radius $R$ having a small circular trap $\Omega_\delta = |\mathbf{x}| \le \delta$. The concentration with $\mathbf{x} = (x, y)$, where $|x| < L$ and $|y| < \pi R$, satisfies

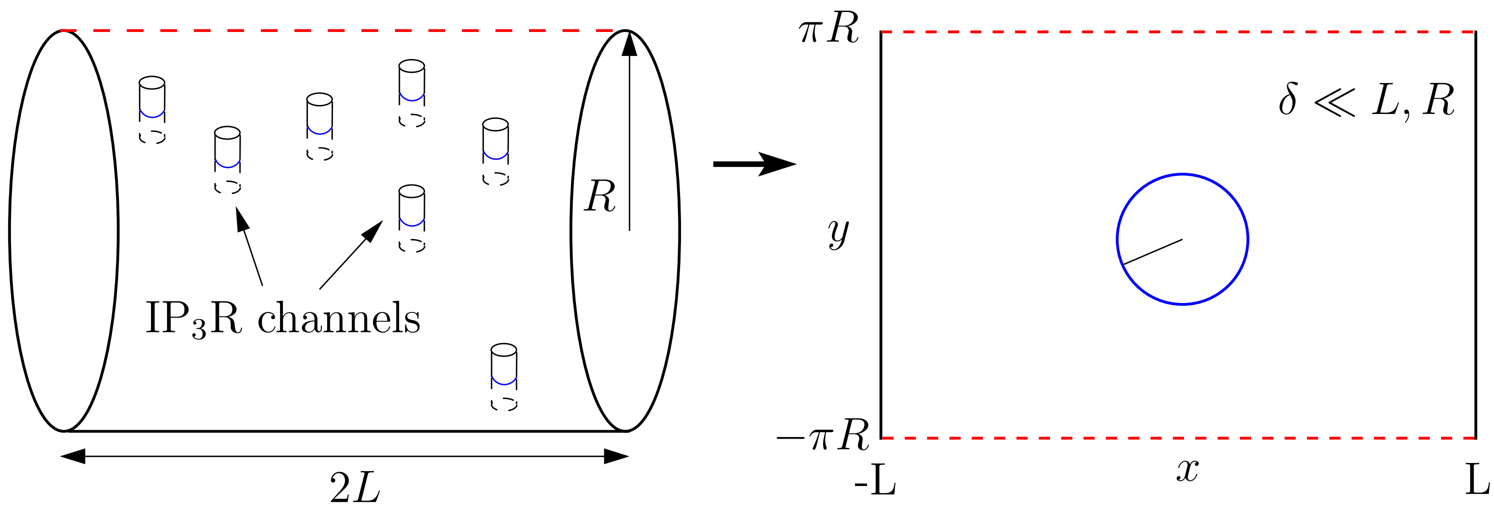
$$c_t = D\Delta c\,, \quad \mathbf{x} \in \Omega \backslash \Omega_\delta\,,$$

$$\partial_x c = 0\,, \quad x = \pm L\,; \quad c,\ \partial_y c\,, \quad 2\pi R \text{ periodic in } y\,,$$

$$c = 0\,, \quad \mathbf{x} \in \partial\Omega_\delta\,.$$

Initially, $c(\mathbf{x}, 0) = c_0$. We want to calculate the reaction rate $k(t)$,

$$k(t) = D \int_{\partial\Omega_\delta} \nabla c|_{|\mathbf{x}|=\delta} \cdot \hat{\mathbf{n}}\, dS\,.$$



# Biomembrane Surface Diffusion With Trap II

For $t \gg 1$, then $c(\mathbf{x},t) \sim d_0 \phi_0 e^{-\lambda_0 D t}$, where $d_0 = c_0 \int_{\Omega \setminus \Omega_\delta} \phi_0 \, d\mathbf{x}$. Here $\lambda_0$ and $\phi_0$ are the principal eigenpair of

$$\Delta \phi + \lambda \phi = 0 \,, \quad \mathbf{x} \in \Omega \,; \quad \int_\Omega \phi^2 \, d\mathbf{x} = 1 \,,$$

$$\partial_x \phi = 0 \,, \quad x = \pm L \,; \quad \phi, \ \partial_y \phi \,, \quad 2\pi R \text{ periodic in } y \,,$$

$$\phi = 0 \,, \quad \mathbf{x} \in \partial \Omega_\delta \,.$$

The principal eigenvalue has the following asymptotics for $\delta \ll 1$:

$$\lambda_0 \sim \frac{2\pi\nu}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|} R_m(\mathbf{0};\mathbf{0}) + \frac{8\pi^3\nu^3}{|\Omega|} \left( \left[ R_m(\mathbf{0};\mathbf{0}) \right]^2 - \frac{G_{m2}(\mathbf{0};\mathbf{0})}{|\Omega_0|} \right) \,.$$

Here $\nu = -1/\log \delta$ and $|\Omega| = 4\pi L R$ is the area of the cylindrical surface. The reaction rate is given by

$$k(t) \sim c_0 D \, |\Omega| \ \lambda_0 \, e^{-\lambda_0 D t} \left( 1 - \frac{4\pi^2\nu^2}{|\Omega|} G_{m2}(\mathbf{0};\mathbf{0}) \right) \,.$$

# Biomembrane Surface Diffusion With Trap III

The Neumann Green's function $G_m(\mathbf{x};\mathbf{0})$ with regular part $R_m(\mathbf{0};\mathbf{0})$ satisfy

$$\Delta G_m = \frac{1}{|\Omega|} - \delta(\mathbf{x}) \, ; \quad \int_\Omega G_m \, d\mathbf{x} = 0 \, ,$$

$$\partial_x G_m = 0 \, , \quad x = \pm L \, ; \quad G_m, \; \partial_y G_m \, , \quad 2\pi R \text{ periodic in } y \, ,$$

$$G_m(\mathbf{x};\mathbf{0}) \sim -\frac{1}{2\pi} \log|\mathbf{x}| + R_m(\mathbf{0};\mathbf{0}) \quad \text{as } \mathbf{x} \to \mathbf{0} \, .$$

With the same boundary conditions, $G_{m2}(\mathbf{x};\mathbf{0})$ satisfies

$$\Delta G_{m2} = -G_m \, ; \quad \int_\Omega G_{m2} \, d\mathbf{x} = 0 \, .$$

Clearly, $G_m$ has the Fourier series representation

$$G_m(\mathbf{x};\mathbf{0}) = \frac{2}{|\Omega|} \left( \frac{1}{\pi^2} \sum_{m=1}^{\infty} \frac{\cos(m\pi x)}{m^2} + \frac{R^2}{L^2} \sum_{n=1}^{\infty} \frac{\cos\left(\frac{nL}{R} y\right)}{n^2} \right)$$

$$+ \frac{2}{|\Omega|} \sum_{m,n=1}^{\infty} \frac{2\cos(m\pi x)\cos\left(\frac{nL}{R} y\right)}{(m\pi)^2 + \left(\frac{nL}{R}\right)^2} \, .$$

# Biomembrane Surface Diffusion With Trap IV

By using Ewald-type summation techniques to extract $R_m$ from the slowly converging doubly-infinite series we calculate

$$R_m(\mathbf{0};\mathbf{0}) = \frac{1}{2\pi}\left(\frac{L}{6R} - \log\left(\frac{L}{R}\right) - 2\sum_{n=1}^{\infty}\log\left(1 - e^{-2nL/R}\right)\right).$$

The solution $G_{m2}$ has the Fourier series representation

$$\begin{aligned} G_{m2}(\mathbf{x};\mathbf{0}) \quad &= \quad \frac{2}{|\Omega_0^s|}\left(\sum_{m=1}^{\infty}\frac{\cos(m\pi x)}{(\pi m)^4} + \sum_{n=1}^{\infty}\frac{\cos\left(\frac{nL}{R}y\right)}{\left(\frac{nL}{R}\right)^4}\right) \\ &+ \frac{2}{|\Omega_0^s|}\left(\sum_{m,n=1}^{\infty}\frac{2\cos(m\pi x)\cos\left(\frac{nL}{R}y\right)}{\left((m\pi)^2 + \left(\frac{nL}{R}\right)^2\right)^2}\right). \end{aligned}$$

Now, $G_2(\mathbf{0},\mathbf{0})$ is readily evaluated by interchanging the infinite summations with the limiting procedure $\mathbf{x} \to \mathbf{0}$, since the resulting infinite series are absolutely convergent. This gives

$$G_{m2}(\mathbf{0};\mathbf{0}) = \frac{1}{4\pi}\left(\frac{1}{45}\frac{L}{R} + \frac{R}{L}\sum_{n=1}^{\infty}\frac{1}{n^2\sinh^2\left(\frac{L}{R}n\right)} + \frac{R^2}{L^2}\sum_{n=1}^{\infty}\frac{\coth\left(\frac{L}{R}n\right)}{n^3}\right).$$

# Diffusion of Protein Receptors I

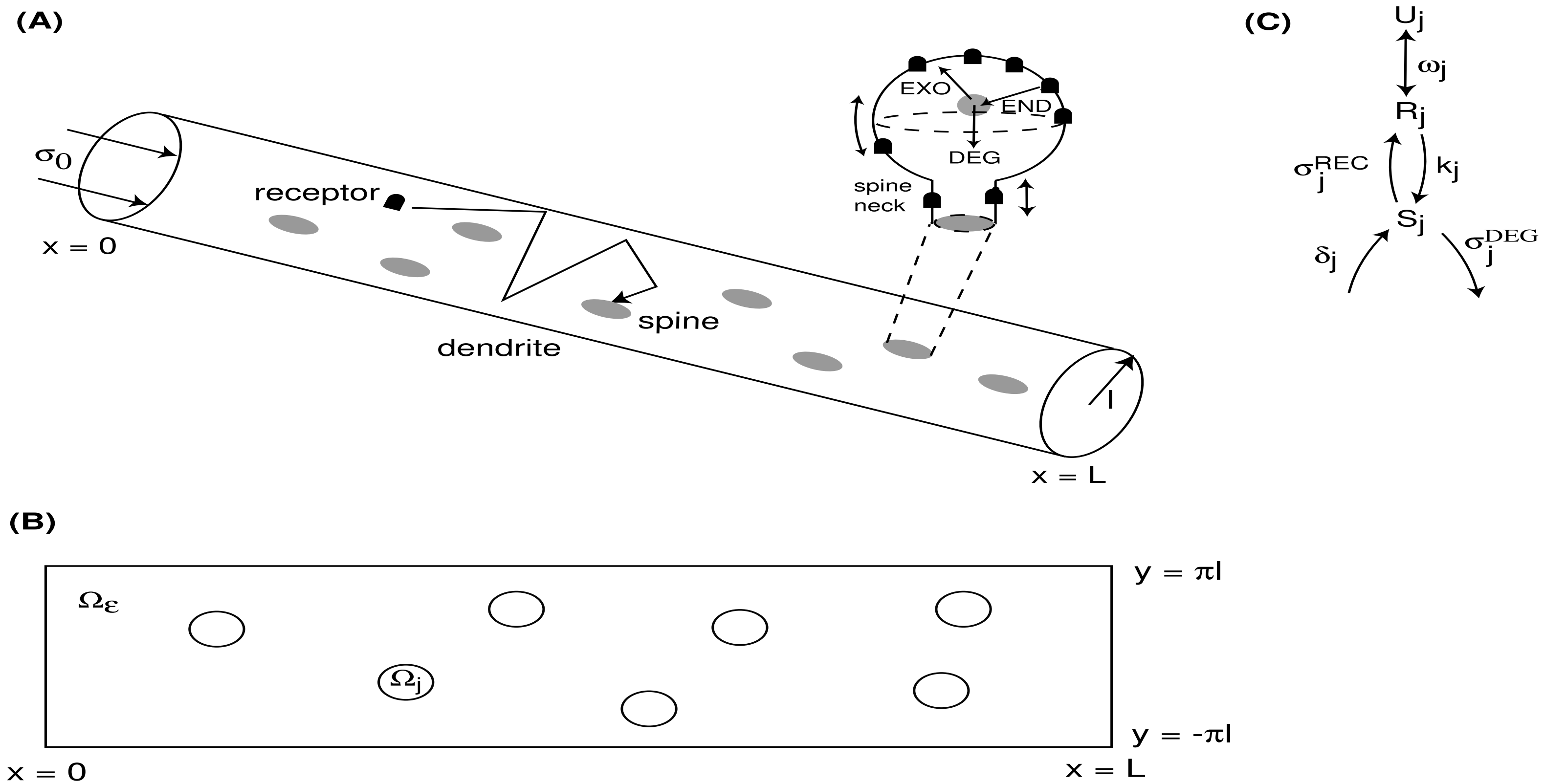
The problem for the diffusion of protein receptors on a cylindrical dendritic membrane $\Omega = \{|x| < L, |y| < 2\pi l\}$, with partially absorbing traps is

$$U_t = \Delta U \,, \quad \mathbf{x} \in \Omega \backslash \Omega_p \,, \quad \Omega_p = \cup_{j=1}^{N} \Omega_{\varepsilon_j} \,,$$

$$\partial_x U(-L, y) = -\sigma \,, \quad \partial_x U(L, y) = 0 \,; \quad U \,, \; \partial_y U \,, \quad 2\pi l \;\text{ periodic in } y \,,$$

$$\varepsilon \partial_n U = -\kappa_j \left( U - T_j \right) \,, \quad \mathbf{x} \in \partial \Omega_{\varepsilon_j} \,, \quad j = 1, \ldots, N \,.$$

Here $\sigma > 0$ models the influx of protein receptors from the soma.



# Diffusion of Protein Receptors II

Define the average concentration $U_j$ on the boundary of the $j^{\text{th}}$ spine

$$U_j = \frac{1}{2\pi\varepsilon} \int_{\partial\Omega_{\varepsilon_j}} U \, d\mathbf{x} \, .$$

Within each spine $T_j(t)$ and $S_j(t)$ for $j = 1, \ldots, N$ satisfy coupled ODE's of the form

$$T_j^{'} = \mathcal{F}_j \left(T_j, S_j, U_j\right) \, , \qquad S_j^{'} = \mathcal{H}_j \left(T_j, S_j\right) \, .$$

- This model is due to Bressloff and Earnshaw (Phys. Rev. E. (2007), J. Neuroscience (2006)). The 1-D problem was studied by them.
- Calculation of the steady-state solution in terms of $\sigma$ and the locations of the dendritic spines.
- Stability analysis: couples the stability of ODE's within each spine to the stability problem for the "outer" diffusion equation.
- Time dependent computations?

# Diffusion of Protein Receptors III

The 2-D steady-state problem fits in the same framework as the other problems. Define $\mathcal{U}$ by

$$\mathcal{U} = U - U_c(x)\,, \qquad U_c(x) = \frac{\sigma}{2L}(x-L)^2\,.$$

With $\nu = -1/\log\varepsilon$. By using inner-outer matching, $\mathcal{U}$ satisfies

$$\Delta\mathcal{U} = -\frac{\sigma}{L}\,, \quad \mathbf{x}\in\Omega\backslash\Omega_p\,,$$

$$\partial_x\mathcal{U}(\pm L, y) = 0\,; \quad \mathcal{U}\,,\ \partial_y\mathcal{U}\,, \quad 2\pi l \text{ periodic in } y\,,$$

$$\mathcal{U} \sim \nu A_j \log|\mathbf{x}-\mathbf{x}_j| + A_j + U_j - U_c(x_j)\,, \quad \text{as } \mathbf{x}\to\mathbf{x}_j\,.$$

The solution in terms of $G_m$ is $\mathcal{U} = -2\pi\nu\sum_{j=1}^{N} A_j G_m(\mathbf{x};\mathbf{x}_j) + \chi$. Then, we obtain $2N+1$ equations for the unknowns $A_j$, $U_j$ and $\chi$:

$$2\pi\nu\sum_{j=1}^{N} A_j = \frac{\sigma}{L}|\Omega|\,, \quad \text{(Divergence Theorem)}\,,$$

$$(1+2\pi\nu R_{mjj})\,A_j + 2\pi\nu\sum_{i\neq j} A_i G_{mji} = U_c(x_j) - U_j + \chi\,, \quad \text{(Point constraint)}$$

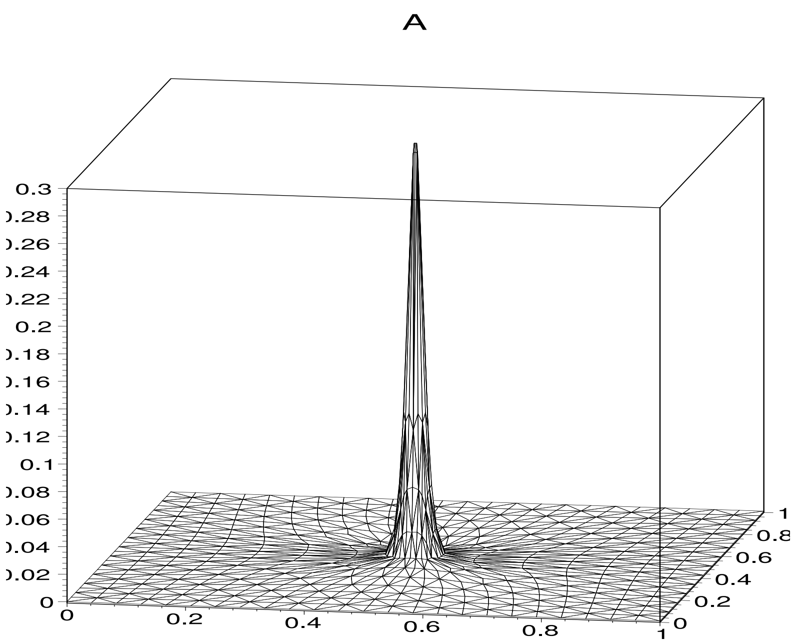
$$2\pi\nu A_j = \kappa_j(U_j - T_j)\,, \quad \text{(BC on each trap)}\,.$$

# Spot Stability for the GM Model

The activator $a$ and inhibitor $h$ in a 2-D domain $\Omega$, with $\varepsilon \ll 1$ satisfy

$$a_t = \varepsilon^2 \triangle a - a + \frac{a^2}{h}, \quad \partial_n a = 0, \quad x \in \partial\Omega$$
$$\tau h_t = D \triangle h - h + \varepsilon^{-2} a^2, \quad \partial_n h = 0, \quad x \in \partial\Omega.$$

The problem has no variational structure. There are particle-like solutions for $a$, called spots, when $\varepsilon \ll 1$. Since $a$ is localized, $\varepsilon^{-1} a^2 \to \sum_{j=1}^{N} S_j \delta(x - x_j)$ in the "outer" region. Hence, the "outer" equilibrium problem for $h$ is solvable by Green's functions.



# Spot Stability for the GM model: I

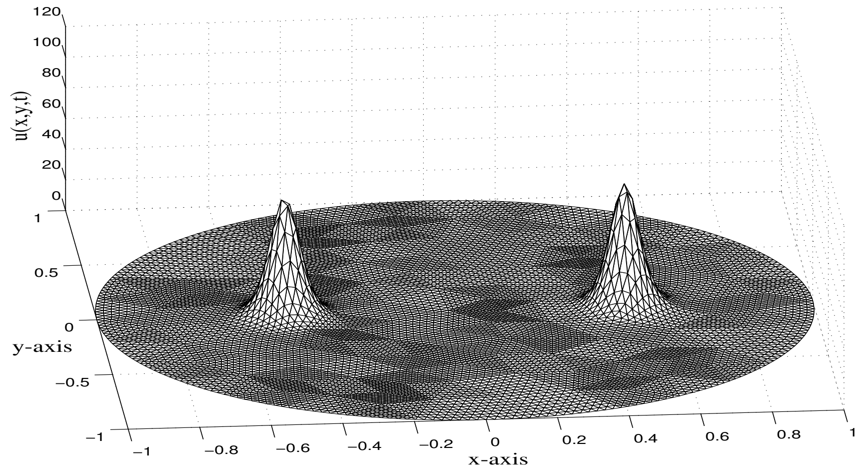
By analyzing a leading order nonlocal eigenvalue problem (NLEP):

**Theorem:** [Winter, Wei, JNLS 2001] For $\tau = 0$, $\varepsilon \to 0$, and $D \geq O(-\ln \varepsilon)$, an $N$-spot equilibrium solution is stable on an $O(1)$ time-scale iff

$$D < D_N \sim \frac{|\Omega|}{2\pi\nu N}, \qquad \nu \equiv -1/\ln \varepsilon\,.$$

- This leading-order term in a logarithmic expansion predicts that $D_N$ is independent of the spot locations $x_j$, $j = 1, \ldots, N$.
- We need higher order terms in the logarithmic series for $D_N$. As for the Neumann eigenvalue problem with traps, we anticipate

$$D_N \sim \frac{|\Omega|}{2\pi\nu N} + F(x_1, \ldots, x_N) + O(\nu)\,, \quad \nu \equiv -1/\ln \varepsilon\,.$$




For a movie showing a spike collapse due to overcrowding click here.

# Spot Stability for the GM model: II

Upon including the next term in the logarithmic series for the stability analysis:

**Principal Result:** [KW, 2006] Let $\tau = 0$, $\varepsilon \to 0$, $D \geq O(\nu^{-1})$ where $\nu \equiv -1/\ln\varepsilon$. Then, an $N$-spot quasi-equilibrium solution is stable on an $O(1)$ time-scale iff

$$D < D_N \sim \frac{|\Omega|}{2\pi\nu N} + |\Omega| \left( -p(x_1, \ldots, x_N) + \frac{2}{N} \min_{j=1,\ldots,N-1} \boldsymbol{c}_j^t \mathcal{G} \boldsymbol{c}_j \right) + O(\nu) \,.$$

Here $\boldsymbol{e}^t = (1, \ldots, 1)$ and the $\boldsymbol{c}_j$ correspond to an $N-1$ dimensional subspace perpendicular to $e$: i.e. $\boldsymbol{c}_j^t e = 0$ for with $\boldsymbol{c}_j^t \boldsymbol{c}_j = 1$.

**Sketch:** Let $w$ be the radially symmetric ground state solution for the spatial profile of the activator. The NLEP problems for $\tau = 0$ are

$$\triangle\Phi - \Phi + 2w\Phi - \chi_j w^2 \frac{\int_{\mathbb{R}^2} w\Phi \, dy}{\int_{\mathbb{R}^2} w^2 \, dy} = \lambda\Phi \,, \quad j = 1, \ldots, N \,,$$

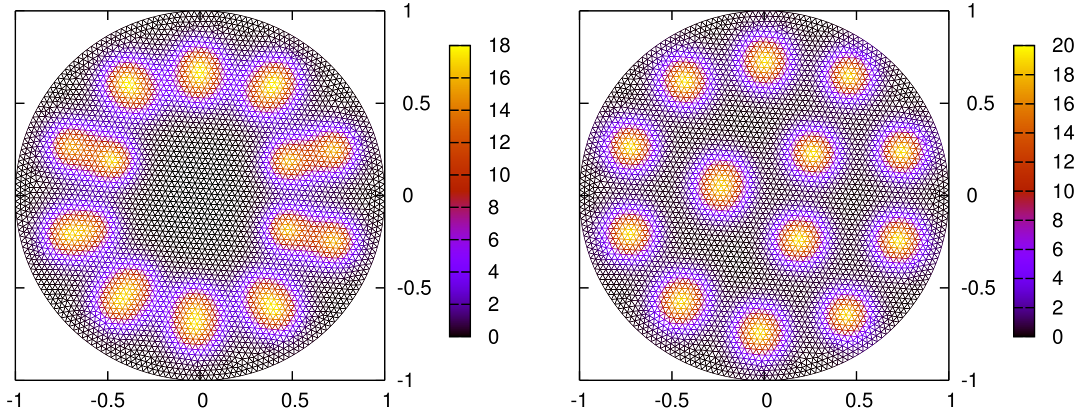
$$\chi_j \equiv \frac{2N\mu_j}{\boldsymbol{e}^t \mathcal{G} \boldsymbol{e}} \,, \qquad \mathcal{C}\boldsymbol{c}_j = \mu_j \boldsymbol{c}_j \,, \qquad \mathcal{C} \equiv I + \frac{2\pi\nu D}{|\Omega|} \boldsymbol{e}\boldsymbol{e}^t + 2\pi\nu\mathcal{G} \,.$$

To calculate the stability threshold set $\min \chi_j = 1$ and solve for $D = D_N$.

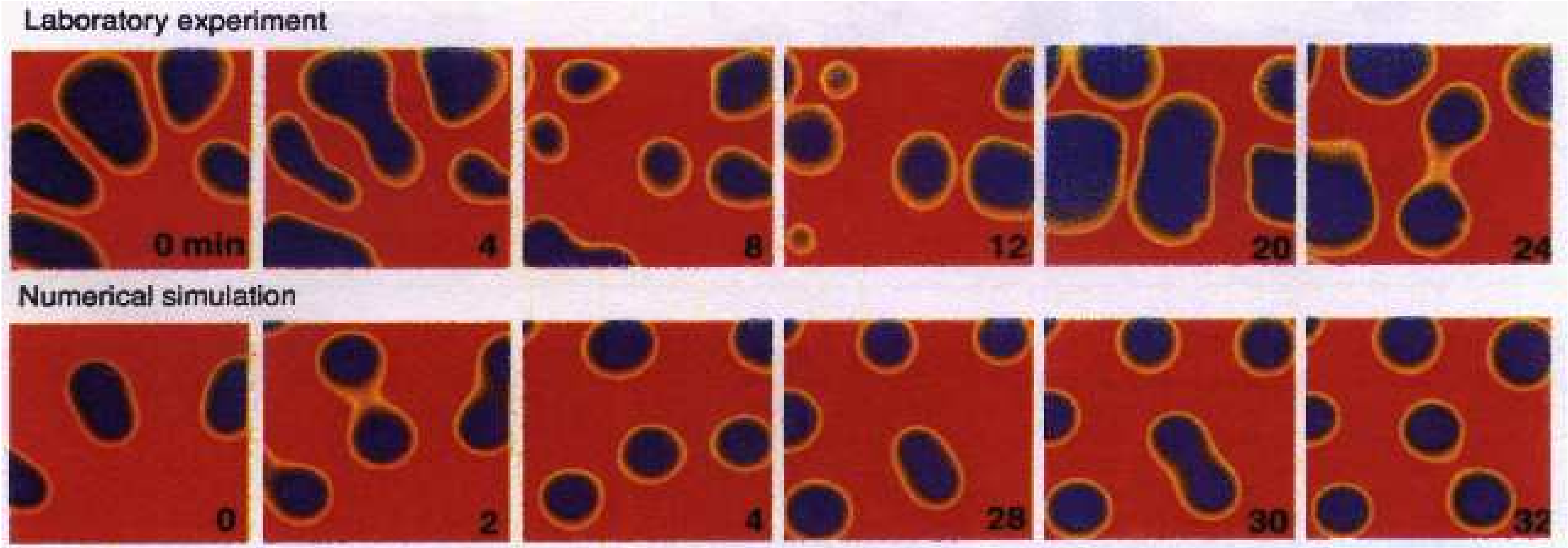
# Spot Replication for the Gray-Scott Model: I

$$v_t = \varepsilon^2 \triangle v - v + A u v^2 \,, \quad \tau u_t = D \triangle u - (1-u) - u v^2 \,.$$

Spot splitting: 2-D GS Model: $A = 3.87$, $D = 1$, $\varepsilon = 0.04$: (Movie)




Exper: FIS Reaction; Numer: GS Model (Swinney et. al. Nature 1994).



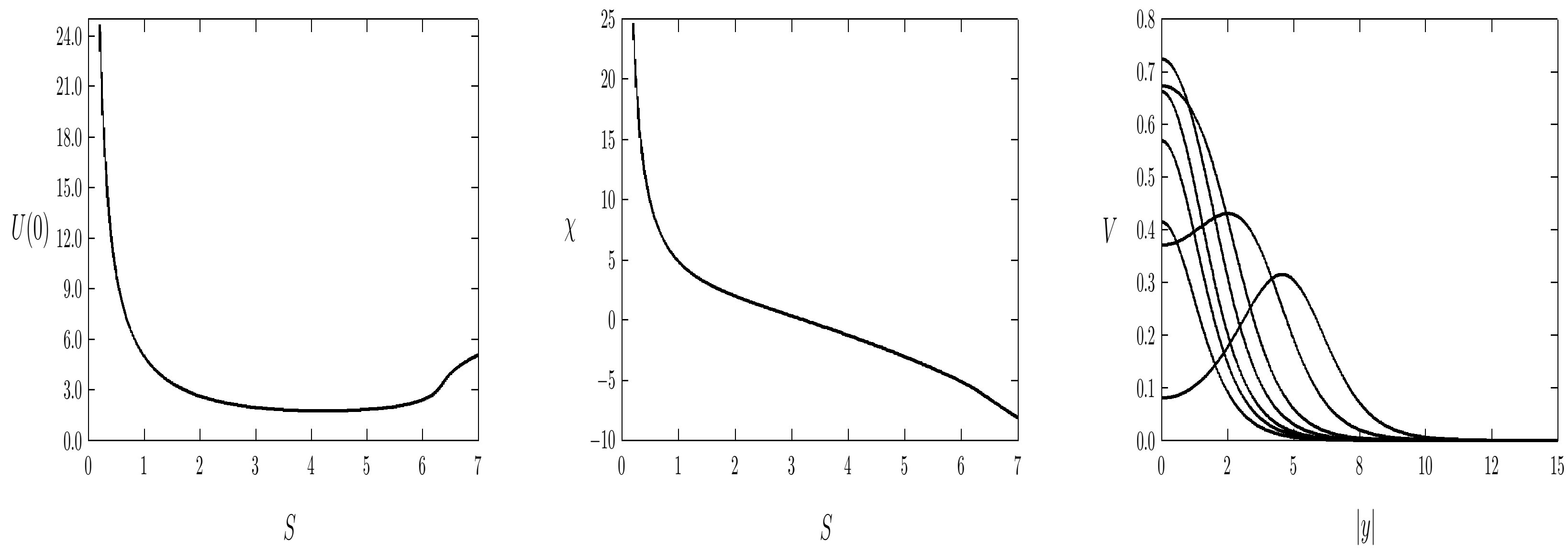
# Spot Replication for the Gray-Scott Model: II

**The Core Solution:** Near the $j^{\text{th}}$ spot we introduce $U$, $V$, and $y$ by $u = \frac{\varepsilon}{A\sqrt{D}} U$, $v = \frac{\sqrt{D}}{\varepsilon} V$, and $y = \varepsilon^{-1}(x - x_j)$. The quasi-steady spatial profile for the $j^{\text{th}}$ spot, referred to as the core problem, is to look for radially symmetric solutions in $\mathbb{R}^2$ to

$$\Delta_y U - UV^2 = 0 \,, \qquad \Delta_y V - V + UV^2 = 0 \,,$$

$$V \to 0 \,, \quad U \sim S_j \log \rho + \chi(S_j) \quad \text{as} \;\; \rho = |y| \to \infty \,.$$

Here $S_j = \int_0^\infty \rho U V^2 \, d\rho$ is a parameter, and $\chi(S_j)$ is to be computed. Notice the volcano pattern for $V$ when $S_j > s_v \approx 4.78$.



# Spot Replication for the Gray-Scott Model: III

**The Outer Problem:** In the “outer” region away from the spots, $uv^2$ is approximated by delta functions. By including all logarithmic terms:

$$\Delta u + \frac{1}{D}(1-u) = \frac{2\pi\nu}{\mathcal{A}} \sum_{j=1}^{N} S_j \delta(x - x_j)\,, \quad x \in \Omega\,; \qquad \partial_n u = 0\,, \qquad x \in \partial\Omega$$

$$u \sim \frac{S_j \nu}{\mathcal{A}} \log|x - x_j| + \frac{1}{\mathcal{A}} \left[S_j + \chi(S_j)\nu\right], \quad \text{as } x \to x_j\,, \quad j = 1, \ldots, N\,.$$

Here $\nu = -1/\log\varepsilon$ and $A$ is related to $\mathcal{A}$ by $A \equiv D^{-1/2}\varepsilon(-\log\varepsilon)\mathcal{A}$.

The point constraint gives $N$ nonlinear algebraic equations for $S_j$:

$$\mathcal{A} = S_j\left(1 + 2\pi\nu R_{jj}\right) + \nu\chi(S_j) + 2\pi\nu \sum_{k\neq j}^{N} S_k G(x_j; x_k)\,, \quad j = 1, \ldots, N\,.$$

Here $R(x;\xi)$ and $G(x;\xi)$ correspond to the Reduced-Wave G-function:

$$\Delta G - \frac{1}{D} G = -\delta(x-\xi)\,, \quad x \in \Omega\,; \qquad \partial_n G = 0\,, \quad x \in \partial\Omega$$

$$G(x,\xi) = -\frac{1}{2\pi}\log|x - x_0| + R(x,\xi)\,.$$

# Spot Replication for the Gray-Scott Model: IV

**Stability to Angular Perturbations:** The stability of the core solution to $e^{im\theta}$ perturbations with $m \geq 2$ is determined by the eigenvalue problem

$$\mathcal{L}_m \Phi - \Phi + 2UV\Phi + V^2 N = \lambda \Phi \,, \quad \Phi \to 0 \,, \quad \text{as } \rho \to \infty \,,$$

$$\mathcal{L}_m N - 2UV\Phi - V^2 N = 0 \,, \quad N \to 0 \,, \quad \text{as } \rho \to \infty \,,$$

$$\mathcal{L}_m \zeta \equiv \zeta'' + \frac{1}{\rho}\zeta' - \frac{m^2}{\rho^2}\zeta \,.$$

Goal: determine critical values $s_m$ of $S_j$ for which we have stability wrt mode $m \geq 2$ iff $S_j < s_m$. Note $N = N(\rho)$ and $\Phi = \Phi(\rho)$.

- We compute numerically that $s_2 \approx 4.31$, $s_3 \approx 5.44$, $s_4 \approx 6.14$. Thus a peanut-splitting instability of the $j^{\text{th}}$ spot will occur when its $S_j$ value satisfies $s_2 < S_j < s_3$. This leads to spot self-replication.
- The spot locations evolve dynamically on a slow (in $\epsilon$) time-scale. Thus, each $S_j$ depends not only on the fixed quantities $\Omega$, $D$, $\mathcal{A}$, but also on all the drifting spot locations $x_j$.
- Thus, a (local) spot-splitting instability can be triggered at some time during the evolution of the collection of spots.

# Spot Replication for the Gray-Scott Model: V

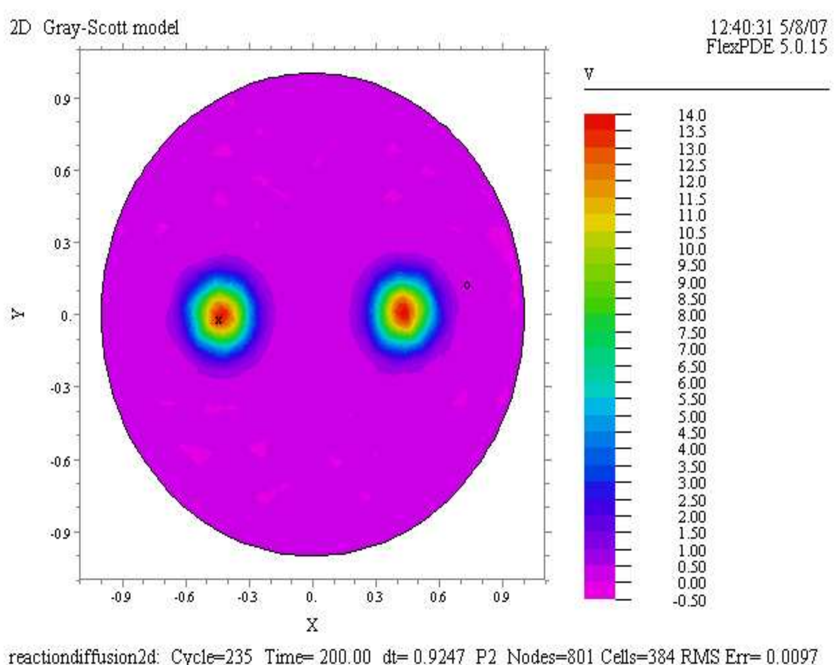
Let $\Omega$ be the unit circle and $\tau = 1$. For $N = 1$ and $x_1 = 0$, we get

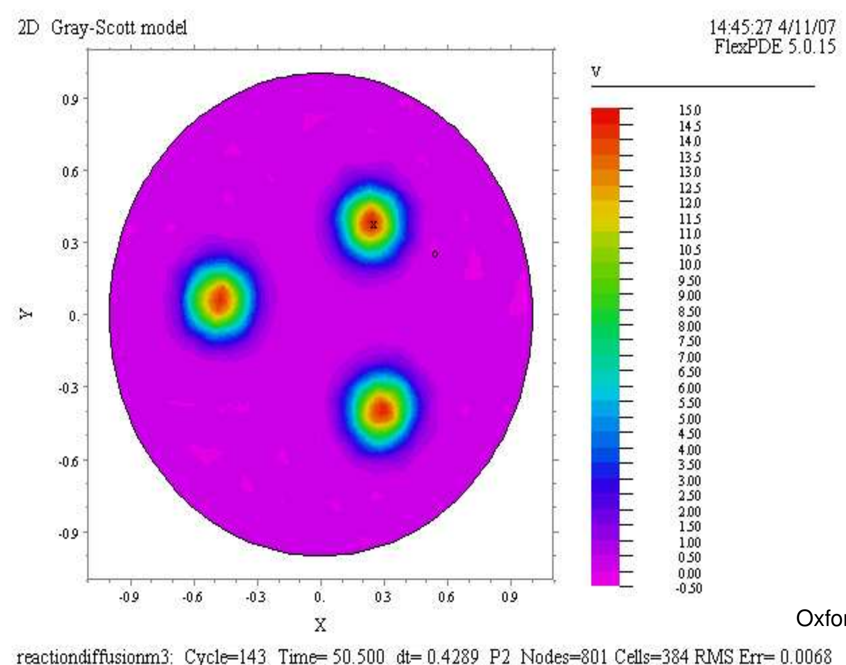
$$R_{11} \equiv R(0;0) = \frac{1}{2\pi}\left[\frac{1}{2}\log D + \log 2 - \gamma - \frac{K_0'(\theta_0)}{I_0'(\theta_0)}\right], \quad \theta_0 = 1/\sqrt{D}\,.$$

Recall that

$$\mathcal{A} = S\left(1 + 2\pi\nu R_{11}\right) + \nu\chi(S)\,.$$

Let $D = 1$ and $\varepsilon = 0.05$. Since $s_2 = 4.31$ and $\chi(s_2) = -1.79$ the spot-splitting threshold is $\mathcal{A}_2 = 5.41$. Similarly $\mathcal{A}_v = 5.79$, and $\mathcal{A}_3 = 6.29$. Full numerics yields a threshold between $\mathcal{A} = 5.6 \sim 5.7$.
(Movie) for $\mathcal{A} = 5.8$. (Movie) for $\mathcal{A} = 7.2$.



# Spot Replication for the Gray-Scott Model: VI

- **NLEP Overcrowding Instability** when $A = O\left[\varepsilon\left(-\log\varepsilon\right)^{1/2}\right]$. A positive real eigenvalue leads to spot-annihilation when there are too many.
- **Spot-Splitting Instability** when $A = O\left[\varepsilon(-\log\varepsilon)\right]$ due to an instability of the core solution the angular mode $m = 2$ (peanut-splitting).
- **Annihilation–Creation Attractors** should be possible since the self-replication and NLEP thresholds are so close in 2-D. Nishiura has observed these numerically in a different parameter regime of the GS model. Imagine that for some spots, $S_j$ exceeds splitting threshold for some $j$. Then spots are created and all the $S_j$ decrease. This gives a smaller effective value of $A$ and we enter NLEP regime, where the spot over-crowding instability occurs. Some spots are destroyed, and the values of $S_j$ increase again.

# Spot Replication: Schnakenburg Model I

The Schnakenburg model in $\Omega$ with no flux BC on $\partial\Omega$ is

$$\nu_t = \varepsilon^2 \triangle \nu + b - \nu + \mu\nu^2 \,, \quad \mu_t = D_u \triangle \mu + a - \mu\nu^2 \,.$$

Let $\nu = \varepsilon^{-2} v$, $\mu = \varepsilon^2 u$, and $D = \varepsilon^2 D_u$. Then,

$$v_t = \varepsilon^2 \triangle v + b\varepsilon^2 - v + uv^2 \,, \quad \varepsilon^2 u_t = D \triangle u + a - \varepsilon^{-2} uv^2 \,.$$

We neglect the $b\varepsilon^2$ term.

- The Schnakenburg model has been used as a prototype RD model to exhibit the effect of pattern generation by domain growth.
- **1-D Patterns:** I. Barrass, E. Crampin, P. Maini (Bull. Math. Bio. 68, (2006)). Mode transitions due to noise.
- **2-D Spots in a Square:** A. Madzvamuse, P. Maini, A. Wathen, (J. Scientific Computing, 24, (2005)). Numerical evidence of spot-splitting.
- Adiabatically slow domain growth of a square or a circle is equivalent to fixing $\Omega$ and decreasing $D$ and $\varepsilon^2$ at the same rate (neglect dilution term).

# Spot Replication: Schnakenburg Model II

Goal: Explain Mode-Doubling in 2-D starting from $N$ Spots:

**The Core Solution:** Near the $j^{\text{th}}$ spot we let $u = \frac{1}{\sqrt{D}} U$, $v = \sqrt{D} V$, and $y = \varepsilon^{-1}(x - x_j)$. We obtain the radially symmetric GS core problem in $\mathbb{R}^2$:

$$\Delta_y U - UV^2 = 0 \,, \qquad \Delta_y V - V + UV^2 = 0 \,,$$
$$V \to 0 \,, \quad U \sim S_j \log \rho + \chi(S_j) \quad \text{as} \;\; \rho = |y| \to \infty \,.$$

**The Outer Problem:** Let $\nu = -1/\log \varepsilon$. The outer problem that accounts for all logarithmic terms is

$$\Delta u = -\frac{a}{D} + \frac{2\pi}{\sqrt{D}} \sum_{j=1}^{N} S_j \delta(x - x_j) \,, \;\; x \in \Omega \,; \quad \partial_n u = 0 \,, \quad x \in \partial\Omega$$
$$u \sim \frac{S_j}{\sqrt{D}} \log|x - x_j| + \frac{1}{\sqrt{D}} \left[ \frac{S_j}{\nu} + \chi(S_j) \right] \,, \quad \text{as} \;\; x \to x_j \,, \;\; j = 1, \ldots, N \,.$$

The solution in terms of the Neumann G-function is

$$u = -\frac{2\pi}{\sqrt{D}} \sum_{j=1}^{N} S_j G_m(x; x_j) + \frac{u_c}{\sqrt{D}} \,.$$

# Spot Replication: Schnakenburg Model III

The point constraints and the div. theorem: $N+1$ equations for $S_j$ and $u_c$

$$\nu u_c = S_j \left(1 + 2\pi\nu R_{mjj}\right) + \nu\chi(S_j) + 2\pi\nu \sum_{k\neq j}^{N} S_k G_m(x_j;x_k)\,, \quad j=1,\ldots,N\,,$$

$$2\pi \sum_{j=1}^{N} S_j = \frac{a}{\sqrt{D}} |\Omega|\,.$$

- For $N=1$, $S_1 = \frac{a|\Omega|}{2\pi\sqrt{D}}$ is independent of $G_m$, $R_m$, and $x_1$. When $S_1 > s_2 = 4.31$, spot-splitting (i.e. mode-doubling) occurs (independent of the spot location $x_1$) when $|\Omega|$ is sufficiently large.
- For $N>1$, we get $u_c = O(\nu^{-1})$, and so $S_j \sim \mathcal{S} + O(\nu)$. Therefore, to leading order in $\nu$, mode-doubling transitions of $N$ spots will occur (approximately) simultaneously when

$$|\Omega| > \frac{2\pi N s_2 \sqrt{D}}{a}\,, \qquad s_2 = 4.31\,.$$

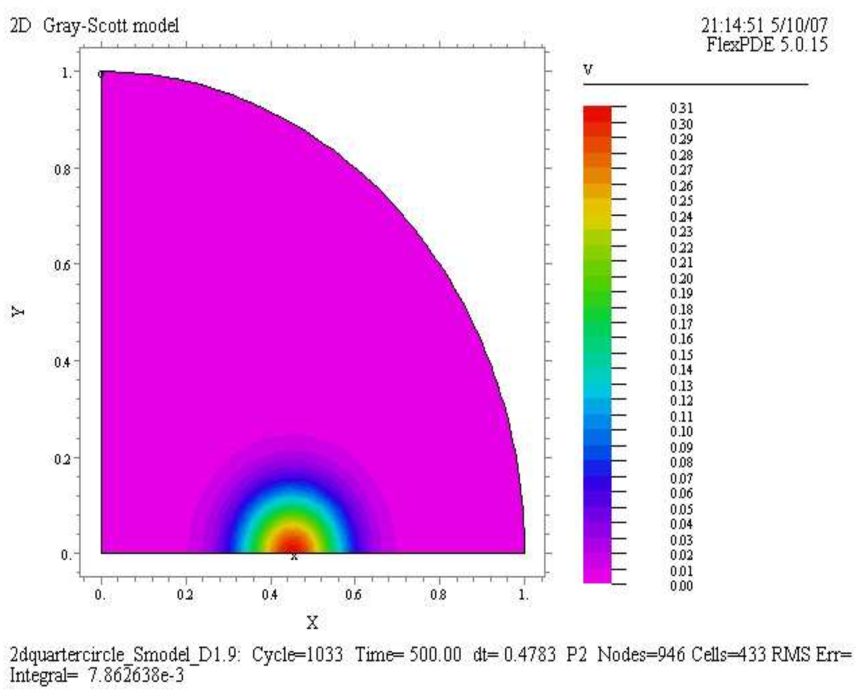
# Spot Replication: Schnakenburg Model IV

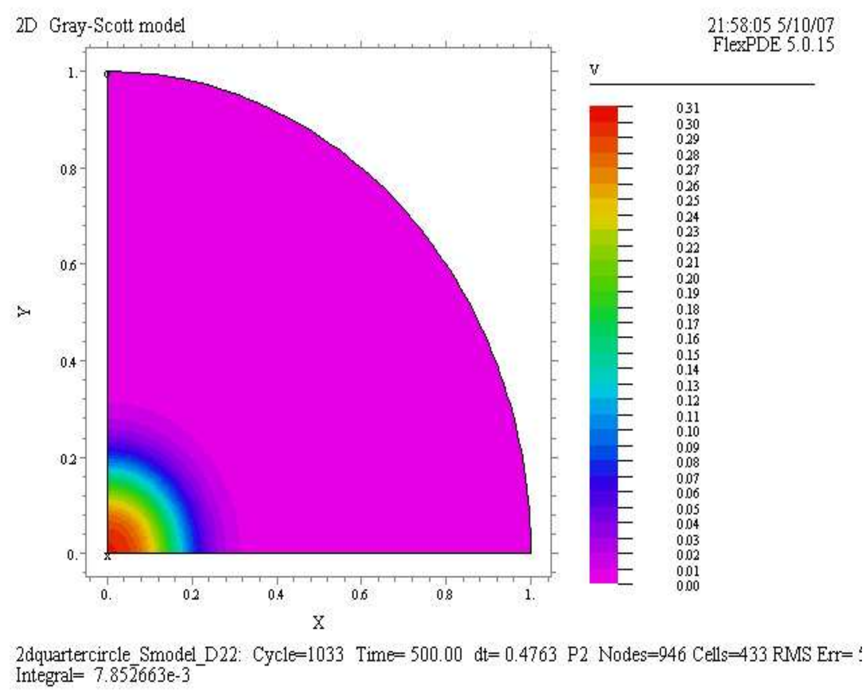
**A Simple Example**

Let $\Omega$ be the unit circle and $a = 4$. Then, starting with one initial spot, a spot-replication event will occur when $D$ crosses below $D_2$ where

$$D_2 = \left(\frac{a|\Omega|}{2\pi s_2}\right)^2 = \left(\frac{a}{2s_2}\right)^2 = \frac{4}{(4.31)^2} = 0.215\,.$$

**Full Numerics:** Left: $D = 0.19$ (split). Right: $D_2 = 0.22$ (split).



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# Dirichlet Green's Function: Regular Part

Consider the Dirichlet Green's function $G_d$, with regular part $R_d$:

$$\triangle G_d = -\delta(x - x_0) \quad x \in \Omega\,; \quad G_d = 0\,, \quad x \in \partial\Omega\,,$$

$$R_d(x, x_0) = G_d(x, x_0) + \frac{1}{2\pi} \log|x - x_0|\,, \qquad \nabla R_{d0} \equiv \nabla R_d(x, x_0)|_{x=x_0}\,.$$

- For a strictly convex domain $\Omega$, $-R_{d0}$ is strictly convex, and thus there is a unique root to $\nabla R_{d0} = 0$. (B. Gustafsson, Duke J. (1990), Caffarelli and Friedman, Duke J. (1985)).
- $\nabla R_{d0}$ can be found for certain mappings $f(z)$ of the unit disk as

$$f'(z_0)\nabla R_{d0} = -\frac{1}{2\pi}\left(\frac{z_0}{1 - |z_0|^2} + \frac{f''(\overline{z}_0)}{2f'(\overline{z}_0)}\right)\,.$$

- Let $B$ be the unit disk and $f(z) = \frac{(1-a^2)z}{z^2-a^2}$. Then $f(B)$ is a symmetric nonconvex dumbbell domain for $1 < a < 1 + \sqrt{2}$. Gustafson (1990) proved that $\nabla R_{d0} = 0$ has three roots when $1 < a < \sqrt{3}$.
- Can one derive a similar result for the Neumann Green's function?

# An Explicit Formula for $\nabla R_{m0}$

**Theorem: (KW)** Let $f(z)$ map the unit disk $B$ onto $\Omega$ satisfying:

(i) $f$ is analytic and is invertible on $\overline{B}$, with $\overline{f(z)} = f(\overline{z})$.

(ii) $f$ has only simple poles at $z_1, .., z_k$, and $f$ is bounded at $\infty$.

(iii) $f = g/h$, with $g(z_i) \neq 0$, where $g$ and $h$ are analytic everywhere.

On the image $\Omega = f(B)$, let $R_m$ be the regular part of $G_m$. Then, at $x_0$, with $z_0 \in B$ satisfying $x_0 = f(z_0)$,

$$\nabla R_{m0} = \frac{\nabla s(z_0)}{f'(z_0)}, \quad \nabla s(z_0) = \frac{1}{2\pi}\left(\frac{z_0}{1-|z_0|^2} + \frac{f''(\overline{z}_0)}{2f'(\overline{z}_0)}\right)$$

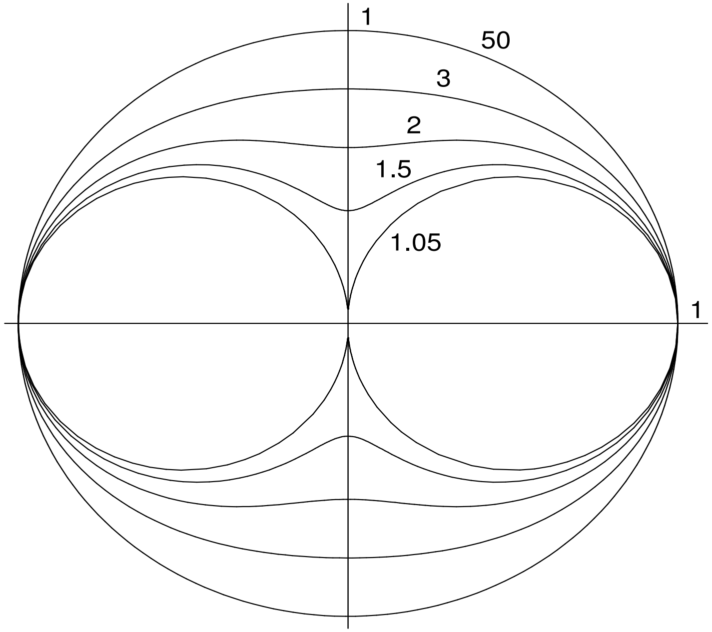
$$-\frac{f'(\overline{z}_0)\left(f(z_0) - f(\frac{1}{\overline{z}_0})\right) + \sum_j \frac{g(z_j)f'(\frac{1}{z_j})}{z_j^2 h'(z_j)}\chi}{2\pi \sum_j \frac{g(z_j)f'(\frac{1}{z_j})}{z_j^2 h'(z_j)}}, \quad \chi = \left(\frac{1}{z_j - \overline{z}_0} + \frac{z_j}{1 - z_j \overline{z}_0}\right)$$

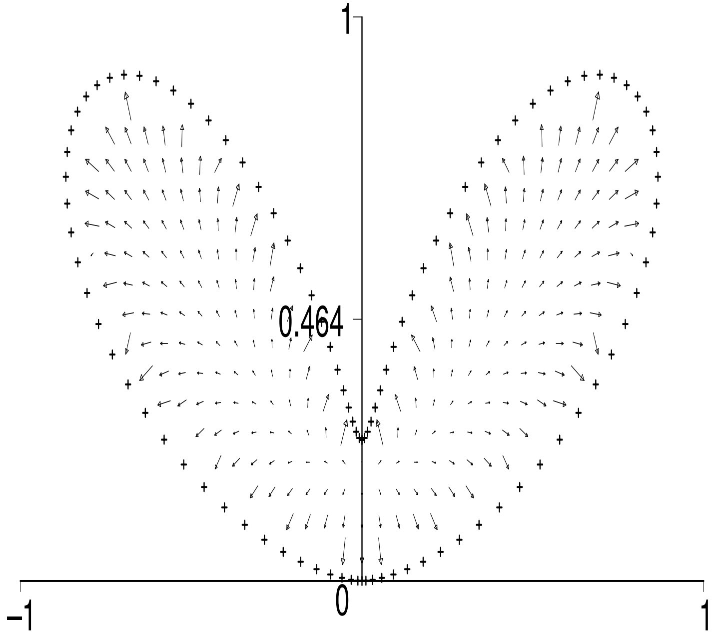
Reference: “Reduced Wave Green’s Functions....”, Kolokolnikov, MJW, EJAM (2003).

# The Zeroes of $\nabla R_{m0}$

**Example 1:** Let $f(z;a) = \frac{(1-a^2)z}{z^2-a^2}$. Then $f(B)$ is nonconvex for $1 < a < 1+\sqrt{3}$. For any $a > 1$, the complex variable formula can be used to show that $\nabla R_{m0} = 0$ has exactly one root at $z = 0$, which maximizes $\lambda_0$ for $\nu \ll 1$. This is qualitatively different than for the Dirichlet problem.

**Example 2:** A boundary integral computes $\nabla R_{m0}$ for other nonconvex symmetric domains. The numerical results give only one root to $\nabla R_{m0} = 0$. The boundary of the domain shown is $(x,y) = (\sin^2 2t + \frac{1}{4}\sin t)(\cos(t), \sin(t)), t \in [0,\pi]$. The vector field $\nabla R_{m0}$ has a unique equilibrium at approximately $(0, 0.2)$.



# A Non-Uniqueness Result I

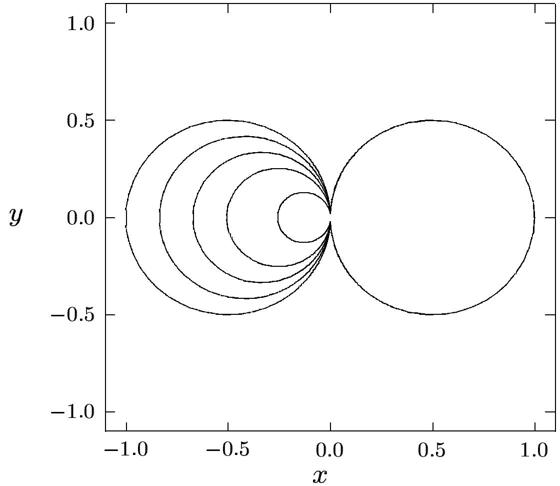
Is there a unique root of $\nabla R_{m0} = 0$ in any simply-connected nonconvex domain? Not necessarily. Let $B$ be the unit ball and $\Omega = f(B)$ where

$$f(z) = -\frac{\kappa z}{(z-a)(z+b)}\,, \quad a = 1+\varepsilon\,, \quad b = 1+\varepsilon\gamma\,,$$

with $\kappa = (a-1)(b+1)$ and $f(1) = 1$. Then, for $\varepsilon \to 0$, the area of $\Omega$ is

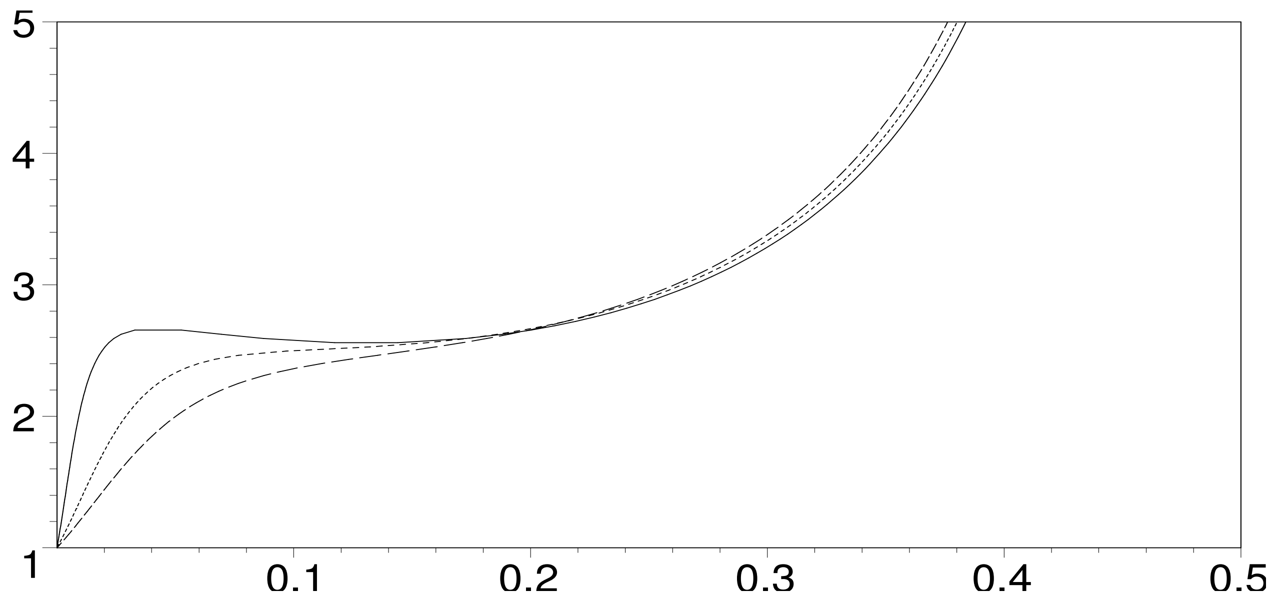
$$|\Omega| \sim \frac{\pi(1+\gamma^2)}{4\gamma^2}\,; \quad \gamma^2 = \text{ratio of area of big lobe to small lobe}$$

Let $\gamma > 1$. For $\varepsilon \to 0$, $\Omega = f(B)$ approaches the union of two circles; a larger circle centred at $(1/2, 0)$ of radius $1/2$, and a smaller circle centred at $(-1/(2\gamma), 0)$ of radius $1/(2\gamma)$. This is an asymmetric dumbbell.



# A Non-Uniqueness Result II

- For $\varepsilon \to 0$, $\nabla R_m = 0$ has a unique root except on $1.5966 < \gamma < \sqrt{3}$.
- For a slightly asymmetric dumbbell, where $1 < \gamma < 1.5966$, the optimum place to maximize $\lambda_0$ is to put the trap in the channel region of the dumbbell, but shifted slightly towards the largest (right) lobe.
- For $\gamma \gg 1$, where the left lobe of the dumbbell is very small the optimum place to insert the trap is near the centre of the right lobe.
- A saddle-node bifurcation structure for $1.5966 < \gamma < \sqrt{3}$ where $\lambda_0$ has two local maxima and a local minimum.




$\gamma^2$ vs. $x_0$ for $\varepsilon = 0.01$ (solid) $\varepsilon = 0.03$ (dotted), and $\varepsilon = 0.05$ (dashed).