Topics in Localized Spot Patterns for Reaction-Diffusion Systems in $\mathbb{R}^2$

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Spots for Singularly Perturbed RD Models

Spatially localized solutions can occur for singularly perturbed RD models

$$v_t = \varepsilon^2 \triangle v + g(u,v)\,; \quad \tau u_t = D \triangle u + f(u,v)\,, \qquad \mathbf{x} \in \Omega \in \mathbb{R}^2\,.$$

Assume semi-strong interactions: $\varepsilon \ll 1$ and $D = \mathcal{O}(1)$.

Key: Since $\varepsilon \ll 1$, v can be localized in space as a spot pattern, i.e. concentration at a discrete set of points.

Prototypical Kinetics: Brusselator, Gray-Scott, GM, Schnakenberg, etc..

Two Distinct Methodologies

- **Classical Approach**: stability of spatially uniform states, Turing and weakly nonlinear analysis of small amplitude patterns, leading to normal form amplitude equations.
- **Localized Patterns:** "Far-from equilibrium patterns" (Nishiura) consisting of "particles" interacting through a "diffusion field".
  - (I) **Key:** $\nu = -1/\log\varepsilon$ is expansion parameter.
  - (II) Spot interactions via Green's functions and Green's matrices
  - (III) Optimization of stability thresholds yield new (discrete) variational problems.

Outline: Spot Stability Analysis for GM Model

The dimensionless (scaled) GM Model in $\Omega_f \in \mathbb{R}^2$ is:

$$v_t = \varepsilon^2 \triangle v - v + v^2/u \,, \quad \partial_n v = 0 \,, \quad \mathbf{x} \in \partial\Omega_f$$
$$\tau u_t = D \triangle u - u + \varepsilon^{-2} v^2 \,, \quad \partial_n u = 0 \,, \quad \mathbf{x} \in \partial\Omega_f \,.$$

- If $D = O(1/\nu) \gg 1$ with $\nu = -1/\log\varepsilon$ linear stability analysis of spot patterns studied through Nonlocal Eigenvalue Problems (NLEPS).
- Competition instability occurs via a zero-eigenvalue crossing. Yields a sign-fluctuating instability of the spot amplitudes.
- Oscillatory instability of the spot amplitudes occurs via a Hopf bifurcation.

Outline:

- **Quasi-Equilibrium:** use SLPT for a quasi-equilibrium spot pattern.
- **Conventional NLEP theory:** Derive the linear stability problem Nonlocal Eigenvalue Problem (NLEP): Recall some well-known spectral results.
- **Extended NLEP theory:**
  - **Hopf bifurcation thresholds:** an anomalous scaling law.
  - **Unfolding a Degenerate zero eigenvalue:** for competition instabilities on a bounded domain and for a periodic pattern in R^2.

Spots: Outline of Theoretical Results

2-D NLEP Stability Theory: $D = \mathcal{O}(\nu^{-1}) \gg 1$ **and** $\nu = -1/\log \varepsilon$

- **Competition Instability Threshold in 2-D Bounded Domains:** Determine the critical value $D_c = \mathcal{O}(\nu^{-1}) \gg 1$ of D for a competition instability.
- **Anomalous Scaling of a HB threshold** for spot amplitude oscillations as τ exceeds a threshold τ_H, with $\tau_H \gg 1$, when $D < D_c$.
- **Refined NLEP theory:** Unfolding the degenerate zero eigenvalue near the leading-order competition threshold D_c.
- **Periodic Patterns:** For a steady-state periodic pattern of spots in $\mathbb{R}^2$ identify the particular lattice arrangement that optimizes the competitition stability threshold. Optimal lattice identified by detailed spectral analysis; no variational principle is available.

Remark: Can extend analysis to other models such as Schnakenberg, Brusselator, and Gray-Scott models.

[W] M. J. Ward, *Spots, Traps, and Patches: Asymptotic Analysis of Localized Solutions to some Linear and Nonlinear Diffusive Processes*, Nonlinearity, **31**(8), (2018), R189 (53 pages). (invited review article).

Overview: NLEP Theory

Key: to leading order in $\nu \equiv -1/\log \varepsilon$ when $D = O(1/\nu)$, the stability theory is based on analysis of nonlocal eigenvalue problems (NLEP's):

$$\Delta \Phi - \Phi + 2w\Phi - \chi(\lambda) w^2 \frac{\int_{\mathbb{R}^2} w\Phi \, dy}{\int_{\mathbb{R}^2} w^2 \, dy} = \lambda \Phi \,.$$

Here $w(\rho) > 0$ is the unique radially symmetric ground state of

$$\Delta_\rho w - w + w^2 = 0 \,, \quad w(0) > 0 \,, \quad w(\infty) = 0 \,, \quad w'(0) = 0 \,.$$

Challenge: NLEP is nonlocal, non-self-adjoint, and $\chi = \chi(\lambda)$. In general χ also depends on N, τ, $|\Omega_f|$, and D.

Basic Theorem (Wei): If $\chi(0) < 1$, and $1/\chi(\lambda)$ analytic in Re$(\lambda) \geq 0$, $\exists$ $\lambda_0 > 0$ real.

Remark: This theorem gives a sufficient condition for instability. Much more challenging to get necessary conditions (Wei-Winter, MJW, etc..)

Quasi-Equilibrium and Linearization

GM Model: Construct an N-spot quasi steady-state pattern (u_e, v_e) with spots of equal height on the finite 2-D domain Ω_f (with Neumann BC), when $D = D_0/\nu \gg 1$ with $\nu = -1/\log \varepsilon \ll 1$:

$$v_t = \varepsilon^2 \triangle v - v + v^2/u\,; \quad \tau u_t = D \triangle u - u + \varepsilon^{-2} v^2\,, \quad \mathbf{x} \in \Omega_f\,.$$

Then, introduce perturbation of the form

$$v = v_e + \sum_{i=1}^{N} c_i e^{\lambda t} \Phi_j \left(\varepsilon^{-1} |\mathbf{x} - \mathbf{x}_i| \right)\,.$$

Remark 1: The coefficients c_i represent amplitude perturbations of the heights of the spots, and are found to satisfy a matrix eigenvalue problem. Unstable eigenvalues in Re$(\lambda) > 0$ with $\lambda = \mathcal{O}(1)$ and $\Phi_j(0) \neq 0$ are referred to as "spot amplitude instabilities" with "mode" $(c_1, \ldots, c_N)^T$:

Remark 2: Derive an eigenvalue problem governing the stability of locally radially symmetric perturbations near each spot. This leads to an NLEP.

. . . . After a detailed asymptotic calculation . . . .

NLEP for Localized Spots of GM: I

NLEP: When $D = D_0/\nu = \mathcal{O}(\nu^{-1})$, with $\nu \equiv -1/\log\varepsilon$, and to leading-order-in-ν the discrete eigenvalues λ of the linearization satisfy:

$$L_0\Psi - \chi_j(\lambda) w^2 \frac{\int_0^\infty w\Psi\rho\,d\rho}{\int_0^\infty w^2\rho\,d\rho} = \lambda\Psi\,, \qquad \Psi \to 0 \quad \text{as} \quad \rho\to\infty\,.$$

Here $L_0 \equiv \Delta_\rho - 1 + 2w$ is the local operator and $w(\rho)$ is the ground-state. The mode $\mathbf{c} = (c_1,\ldots,c_N)^T$ is an eigenvector of the Green's matrix $\mathcal{G}_\lambda$:

$$\mathcal{G}_\lambda \mathbf{c}_j = \kappa_{\lambda,j}\mathbf{c}_j\,, \quad j=1,\ldots,N\,; \qquad (\mathcal{G}_\lambda)_{ij} \equiv \begin{cases} R_{\lambda j} & i=j \\ G_\lambda(\mathbf{x}_i;\mathbf{x}_j) & i\neq j\,. \end{cases}$$

The entries of the eigenvalue-dependent Green's matrix obtained from

$$\Delta G_\lambda - \frac{\nu(1+\tau\lambda)}{D_0} G_\lambda = -\delta(\mathbf{x}-\mathbf{x}_i)\,, \quad \mathbf{x}\in\Omega_f\,; \qquad \partial_n G_\lambda = 0\,, \quad \mathbf{x}\in\partial\Omega_f\,,$$

$$G_\lambda \sim -\frac{1}{2\pi}\log|\mathbf{x}-\mathbf{x}_i| + R_\lambda(\mathbf{x}_i) + o(1) \quad \text{as} \quad \mathbf{x}\to\mathbf{x}_i\,.$$

In terms of κ_j, the multipliers $\chi_j(\lambda)$ for $j=1,\ldots,N$ of the NLEP are

$$\chi_j(\lambda) = \frac{2}{1+\mu}\left(1 + 2\pi\nu\kappa_{\lambda,j}\right)\,, \quad j=1,\ldots,N\,; \quad \mu \equiv \frac{2\pi N D_0}{|\Omega_f|}\,.$$

NLEP for Localized Spots of GM: II

Key Issue: Need to ensure that $\kappa_j = \mathcal{O}(\nu^{-1})$ for self-consistency

Two Ways: (I) Conventional NLEP; (II) New Modified NLEP

Conventional NLEP: Assume $\tau = \mathcal{O}(1)$ and $(1+\tau|\lambda|)\nu/D_0 = \mathcal{O}(\nu)$. Then,

$$\mathcal{G}_\lambda = \frac{D_0 N}{\nu(1+\tau\lambda)|\Omega_f|}\mathcal{E} + \mathcal{G}_0 + \mathcal{O}(\nu)\,, \qquad \mathcal{E} \equiv \frac{1}{N}\mathbf{e}\mathbf{e}^T\,,$$

where $\mathcal{G}_0$ is the Neumann Green's matrix and $\mathbf{e} \equiv (1,\ldots,1)^T$. Since $\mathcal{E}\mathbf{e} = \mathbf{e}$ and $\mathcal{E}\mathbf{q}_j = 0$ where $\mathbf{q}_j^T\mathbf{e} = 0$, then

$$2\pi\nu\kappa_1 \sim \frac{\mu}{1+\tau\lambda}\,; \qquad 2\pi\nu\kappa_j = \mathcal{O}(\nu)\,, \quad \text{for} \quad j = 2,\ldots,N\,.$$

This yields two NLEP multipliers: (synchronous (s), competition (c));

$$\chi_c(\lambda) \equiv \frac{2}{1+\mu}\,, \quad \chi_s(\lambda) = \frac{2}{1+\mu}\left(\frac{1+\mu+\tau\lambda}{1+\tau\lambda}\right)\,; \quad \mu \equiv \frac{2\pi N D_0}{|\Omega_f|}\,.$$

Ref: [WWi,2001] J. Wei, M. Winter, J. Nonlinear Sci., **11**(6), (2001), pp. 415–458.

Conventional NLEP Theory: I

There are N choices for $\boldsymbol{c}_j \equiv (c_1, \ldots, c_N)^T$ (spot amplitude perturbations):

$$\boldsymbol{c}_1 = \boldsymbol{e} \equiv (1, \ldots, 1)^T ; \quad \text{(synchronous)}$$

$$\boldsymbol{c}_j^T \boldsymbol{e} = 0 , \quad j = 2, \ldots, N ; \quad \text{(competition or asynchronous)} .$$

The discrete λ of the NLEP (synchronous) are roots $g(\lambda) = 0$ of

$$g(\lambda) \equiv \frac{1}{\chi_s(\lambda)} - \mathcal{F}(\lambda) , \qquad \mathcal{F}(\lambda) \equiv \frac{\int_0^\infty w \left[(L_0 - \lambda)^{-1} w^2 \right] \rho \, d\rho}{\int_0^\infty w^2 \rho \, d\rho} .$$

Set $\lambda = i\lambda_I$, write $\mathcal{F}(i\lambda_I) = \mathcal{F}_R(\lambda_I) + i\mathcal{F}(\lambda_I)$, and set $g(i\lambda_I) = 0$:

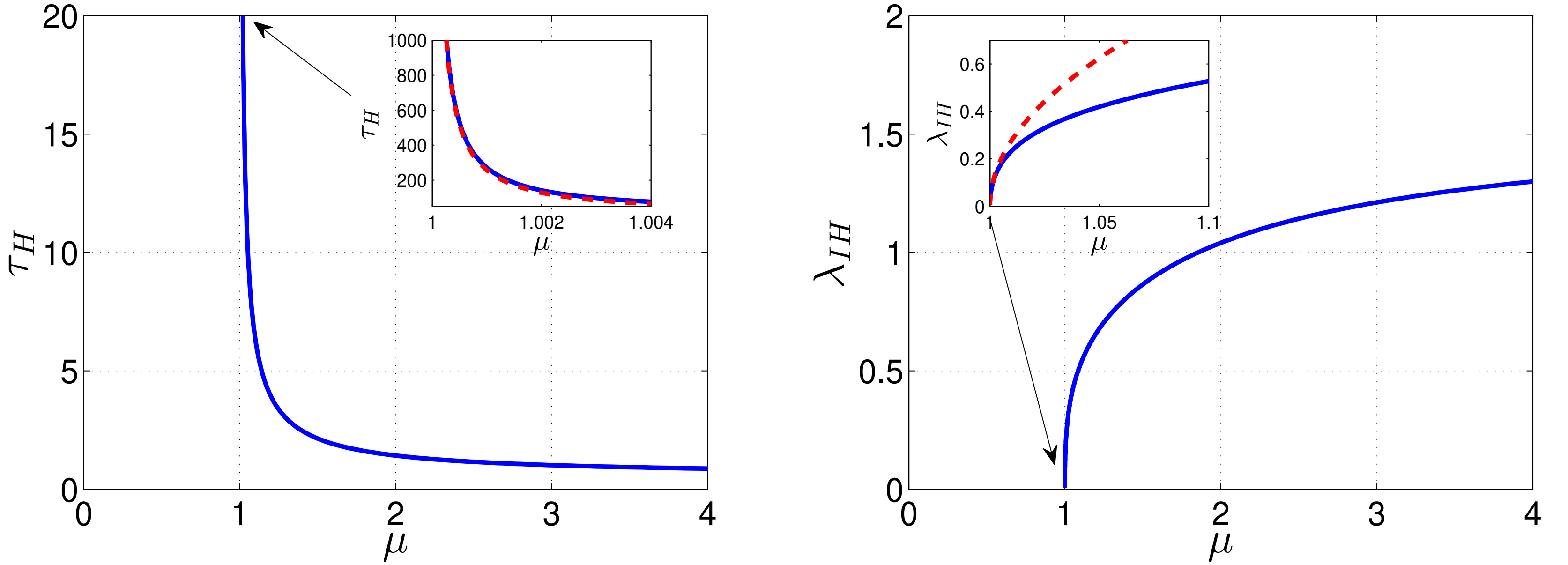
$$\frac{(1+\mu)}{2} \left(\frac{1 + i\tau\lambda_I}{1 + \mu + i\tau\lambda_I} \right) = \mathcal{F}_R(\lambda_I) + i\mathcal{F}_I(\lambda_I) .$$

Separate real and imaginary parts. We get $\mu = \mu(\lambda_I)$ and $\tau_H = \tau_H(\lambda_I)$:

$$\mu = \frac{\left(4|\mathcal{F}|^2 + 1 - \mathcal{F}_R \right)}{2\mathcal{F}_R - 1} , \quad \tau_H = \frac{2|\mathcal{F}|^2 - \mathcal{F}_R}{\lambda_I \mathcal{F}_I} ; \qquad |\mathcal{F}|^2 = \mathcal{F}_R^2 + \mathcal{F}_I^2 .$$

This gives a new parameterization of any HB threshold (**Ref: [TWW]**).

Conventional NLEP Theory: II



Caption: HB threshold τ_H (left) and eigenvalue λ_{IH} (right) vs. μ for the synchronous mode. No HB threshold for $\mu < 1$, and $\tau_H \to +\infty$ while $\lambda_{IH} \to 0^+$ as $\mu \to 1^+$. Inserts validate limiting asymptotics.

With $\kappa_c \approx 0.436$, we obtain the limiting asymptotic behavior

$$\tau_H \sim \frac{2(1-2\kappa_c)}{\mu - 1}, \qquad \lambda_{IH} \sim \sqrt{\frac{\mu-1}{1-2\kappa_c}}, \qquad \text{as} \qquad \mu \to 1^+ .$$

Rigorous: Leading Order NLEP Theory

Main Result (Competition Modes): **[WWi,2001]**: (results independent of τ):

- linearly stable if and only if $\mu < 1$.
- **Key:** to leading order in ν, $N-1$ modes simultaneously go unstable through a zero eigenvalue crossing as μ increases past $\mu = 1$.
- If $\mu = 1$, then $\Phi = w$ and $\lambda = 0$ is an eigenpair of the NLEP.

Main Result (Synchronous Mode): (depends on τ):

- Since $\chi_s(0) = 2$, then $\forall \mu > 0$ and $\forall \tau > 0$ there can be no zero eigenvalue crossings (**[WWi, 2001]**).
- If $\mu > 1$: there is a unique Hopf bifurcation value $\tau_H > 0$. (**[WWi, 2001]**).
- If $0 < \mu < 1$: linearly stable if $0 < \tau < \tau_2$ and if $\tau > \tau_3$, where $\tau_3 \geq \tau_2$ (**[WWi, 2001]**). Unresolved if $\tau_3 > \tau_2$ or $\tau_3 = \tau_2$. Numerics: $\tau_3 = \tau_2$.
- **More recently:** stability $\forall \tau > 0$ with $\tau = \mathcal{O}(1)$ when $0 < \mu < 1$. For $0 < \mu < 1$, Hopf bifurcation stability threshold has anomalous scaling $\tau = \mathcal{O}(\varepsilon^{\mu-1}/\nu) \gg 1$ **[TWW]**.

[TWW] J. Tzou, M. J. Ward, J. Wei, *Anomalous Scaling of Hopf Bifurcation Thresholds for the Stability of Localized Spot Patterns for Reaction-Diffusion Systems in 2-D*, SIADS, **17**(1), (2018), pp. 982-1022.

Leading Order Competition Threshold

Through a rigorous analysis of the Conventional NLEP with multiplier χ_c:

Main Result [WWi,2001]: *Let $N \geq 2$, $\tau = \mathcal{O}(1)$ and consider the NLEP for the competition modes. Then, Re$(\lambda) < 0$ if and only if $D_0 < D_{0c}$. When $D > D_{0c}$, the NLEP has a unique positive real eigenvalue. This leading-order competition threshold is $\mu = 2\pi N D_0/|\Omega_f| = 1$, yielding*

$$D_c = \frac{D_{0c}}{\nu} + \mathcal{O}(1)\,, \qquad D_{0c} \equiv \frac{|\Omega_f|}{2\pi N}\,.$$

Remarks:

- The leading-order threshold is independent of the spot configuration.
- Need to unfold this $N-1$ dimensional zero-eigenvalue crossing to determine refined threshold, i.e. to find the next term

$$D_c \sim \frac{D_{0c}}{\nu} + D_{1c} + \mathcal{O}(\nu)\,.$$

We will do this unfolding for two cases:

- periodic patterns in $\mathbb{R}^2$.
- finite domain Ω_f.

New (Modified) NLEP Problem

Warning: Conventional NLEP (based on $(1+\tau|\lambda|)\nu/D_0 \ll 1$) not valid near D_{0c}.

Question: Does $\exists$ a HB when $D_0 < D_{0c}$ with $\tau \gg 1$?

New (Modified) NLEP: Assume $\tau \gg 1$ such that $|(1+\tau\lambda)\nu/D_0| \gg 1$. Then, G_λ is closely approximated by the free-space Green's function G_f:

$$G_\lambda(\mathbf{x};\mathbf{x}_0) \sim G_f \equiv \frac{1}{2\pi} K_0\left(\theta_\lambda |\mathbf{x}-\mathbf{x}_0|\right) \,, \qquad \theta_\lambda \equiv \sqrt{(1+\tau\lambda)\nu/D_0} \,.$$

Moreover, $\mathcal{G}_\lambda \sim R_\lambda I$, where R_λ is reg. part of G_f. Introduce

$$\tau \equiv \varepsilon^{-\tau_c}/\nu \,, \quad 0 < \tau_c < 2 \,; \qquad \text{(anomalous scaling)} \,.$$

For each j, and with γ_e Euler's constant, we get

$$2\pi\nu\kappa_j = -\frac{\tau_c}{2} + \nu\mathcal{K}_\varepsilon \,, \qquad \mathcal{K}_\varepsilon \equiv -\frac{1}{2}\log(\lambda + \nu\varepsilon^{\tau_c}) + \log\left(2\sqrt{D_0}\right) - \gamma_e \,.$$

The discrete eigenvalues of the NLEP are the roots of $g(\lambda) = 0$ where

$$g(\lambda) \equiv \frac{(1+\mu)}{2}\left(1 - \frac{\tau_c}{2} + \nu\mathcal{K}_\varepsilon\right)^{-1} - \mathcal{F}(\lambda) \,.$$

Anomalous Scaling of a HB: I

To determine a HB we set $g(i\lambda_I) = 0$ and calculate τ_c. Notice that $g(0) = 0$ when $\tau_c = 1 - \mu$ and $\nu = 0$.

Fix μ in $0 < \mu < 1$ and separate into real and imaginary parts:

$$\tau_c - (1-\mu) = (\tau_c - 2)\left[1 - \text{Re}(\mathcal{F}(i\lambda_I))\right] + 2\nu \text{Re}\left[\mathcal{K}_\varepsilon \mathcal{F}(i\lambda_I)\right] ,$$

$$(\tau_c - 2)\lambda_I = 4\nu \text{Im}\left[\mathcal{K}_\varepsilon \mathcal{F}(i\lambda_I)\right] .$$

We then use $\mathcal{F}(i\lambda_I) \sim 1 + \frac{i\lambda_I}{2} - \kappa_c \lambda_I^2 + \ldots$ for $\lambda_I \ll 1$.

Main Result: [TWW] *Let $D_0 < D_{0c}$, ($\mu < 1$), $\varepsilon \ll 1$ with $\nu = -1/\log \varepsilon$. Then, the modified NLEP has a HB corresponding to temporal oscillations in the spot amplitudes, when $\tau = \tau_H \gg 1$ and $\lambda = \pm i\lambda_I$, with anomalous scaling:*

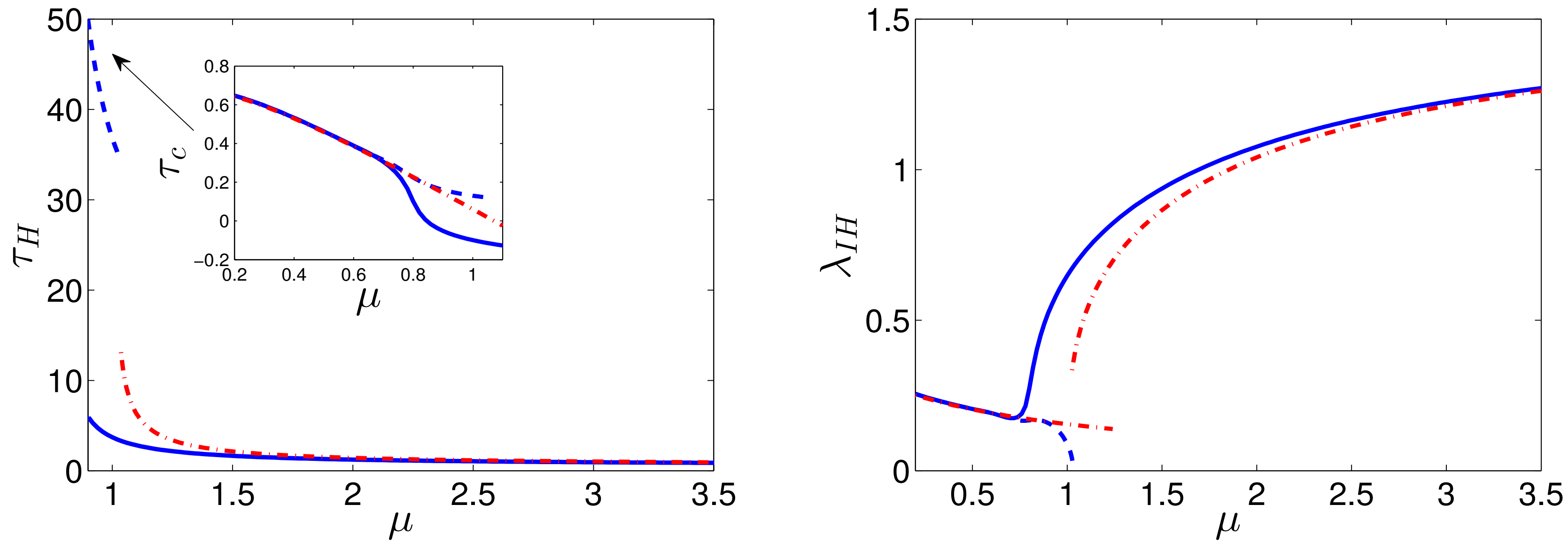
$$\tau_H \sim \frac{1}{\nu}\varepsilon^{-\tau_c} ; \qquad \tau_c = (1-\mu) - \nu \log \nu + (2\beta - \log \lambda_{I0})\, \nu + \mathcal{O}(\nu^2) ,$$

$$\lambda = i\nu \left[\lambda_{I0} + \nu \frac{\pi^3}{(1+\mu)^3}\left(\frac{1}{4} - 2\kappa_c\right)\right] + \mathcal{O}(\nu^3) ,$$

where $\lambda_{I0} = \pi/(1+\mu)$, $\beta \equiv \log\left(2\sqrt{D_0}\right) - \gamma$, and $\kappa_c \approx 0.436$.

Anomalous Scaling of a HB: II

- The anomalous HB threshold is (asymptotically) the same $\forall j$. τ_c is independent of spot locations. Spatial mode spans $\mathbb{R}^N$.
- Not uniformly valid as $D_0 \to D_{0c}^-$. For D_0 near D_{0c} we need NLEP with multipliers χ_j in terms of "full" Green's matrix $\mathcal{G}_\lambda$ and its "full" matrix spectra κ_j. For D_0 near D_{0c}, spot configuration for HB is important. Matrix eigenvectors give distinct instability modes for spot amplitudes.



Caption: HB threshold τ_H (left) and eigenvalue λ_{IH} for a two-spot ring pattern in the unit disk for $r_0 = 0.452$ and $\nu = 0.1$. Solid (Dashed): synchronous (asynchronous) mode from full NLEP. Dot-dashed curves: for $\mu > 1$ are conventional NLEP theory and for $\mu < 1$ from scaling law

Periodic Problem: Unfolding $\lambda = 0$: I

Summary: On Ω_f, we have linear stability $\forall \tau > 0$ with $\tau = \mathcal{O}(1)$, when

$$D < D_c \sim \frac{D_{0c}}{\nu}\,, \qquad D_{0c} \equiv \frac{|\Omega_f|}{2\pi N}\,, \qquad \nu = -1/\log\varepsilon\,.$$

Motivation: Consider periodic pattern of spots in $\mathbb{R}^2$ concentrated at lattice points of Bravais lattice. Effectively, $|\Omega_f| \to N|\Omega|$, where $|\Omega|$ is the area of a Wigner Seitz cell. Consider the "blow up:"

$$D = \frac{|\Omega|}{2\pi\nu}\left(1 + \mu_1 \nu\right) + o(1)\,, \quad \mu_1 = \mathcal{O}(1) \text{ is a "de-tuning parameter"}\,,$$

- Calculate the band of continuous spectrum satisfying $|\lambda| = \mathcal{O}(\nu) \ll 1$.
- For a given lattice Λ, choose μ_1 sufficiently small so that the entire band satisfies Re$(\lambda) < 0$.
- Fix $|\Omega| = 1$. Maximize μ_1 with respect to Λ, to identify the "optimal" lattice that allows for stability for the largest range of D.

[IRWW, 2014] Iron, Rumsey, Ward, Wei, *Logarithmic expansions and the Stability of Periodic Patterns of Localized Spots for RD Systems in* $\mathbb{R}^2$, J. Non. Sci., **24**(5), (2014), pp. 857–912.

A Primer on Lattices: I

We will consider the class of Bravais lattices Λ defined by

$$\Lambda \equiv \left\{ m\boldsymbol{l}_1 + n\boldsymbol{l}_2 \,\middle|\, m,\, n \in \mathbb{Z} \right\}.$$

WLOG, align $\boldsymbol{l}_1$ with positive x-axis.

Primitive cell: parallelogram generated by the vectors $\boldsymbol{l}_1$ and $\boldsymbol{l}_2$.

Wigner Seitz cell centered at $\boldsymbol{l} \in \Omega$ is the set of all points closer to $\boldsymbol{l}$ than any other lattice point (Voronoi cell)

- The union of the WS cells tile $\mathbb{R}^2$.
- The Fundamental WS cell Ω (FWS) is centered at the origin. We set $|\Omega| = 1$. Note: $|\Omega| = |\boldsymbol{l}_1 \times \boldsymbol{l}_2|$.

For a regular hexagonal lattice with $|\Omega| = 1$, we have

$$\boldsymbol{l}_1 = \left(\left(\frac{4}{3}\right)^{1/4}, 0 \right) \qquad \text{and} \qquad \boldsymbol{l}_2 = \left(\frac{4}{3}\right)^{1/4} \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right).$$

A Primer on Lattices: II

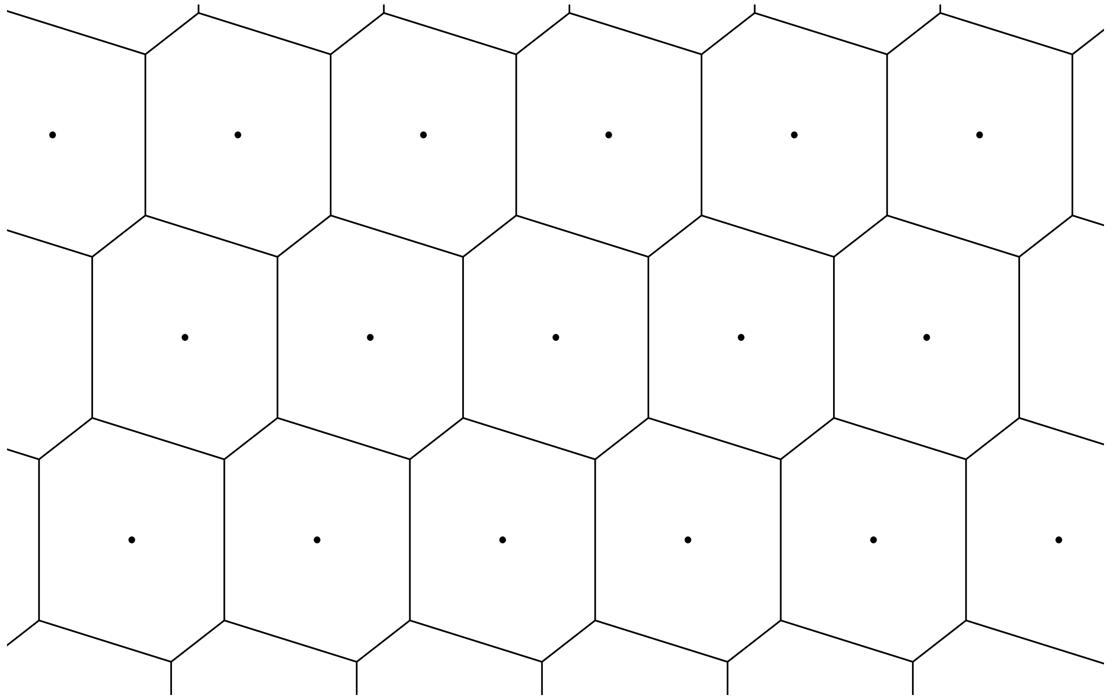


Figure 1: WS cells for an oblique lattice with $\boldsymbol{l}_1 = (1,0), \boldsymbol{l}_2 = (\cot\theta, 1)$, and $\theta = 74°$, so that $|\Omega| = 1$. These cells tile the plane.

- Generically, the FWS cell has three pairs of parallel sides of equal length (except for rectangular cells).
- Triangular lattices are excluded since we cannot tile $\mathbb{R}^2$ with translates of a FWS.

A Primer on Lattices: III

Reciprocal lattice: $\Lambda^\star$ is defined in terms of two independent vectors $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, satisfying

$$\boldsymbol{d}_i \cdot \boldsymbol{l}_j = \delta_{ij}\,, \qquad \Lambda^\star \equiv \left\{ m\boldsymbol{d}_1 + n\boldsymbol{d}_2 \,\middle|\, m,\, n \in \mathbb{Z} \right\}.$$

First Brillouin zone Ω_B**:** is the Fundamental WS cell in reciprocal space.

Poisson Summation Formula (PSF) between direct and reciprocal lattices:

$$\sum_{\boldsymbol{l}\in\Lambda} f(\mathrm{x}+\boldsymbol{l})\, e^{i\boldsymbol{k}\cdot\boldsymbol{l}} = \frac{1}{|\Omega|} \sum_{\boldsymbol{d}\in\Lambda^*} \hat{f}(2\pi\boldsymbol{d}-\boldsymbol{k})\, e^{i\mathrm{x}\cdot(2\pi\boldsymbol{d}-\boldsymbol{k})}\,, \qquad \boldsymbol{k}/(2\pi) \in \Omega_B\,,$$

where $\hat{f}$ is the Fourier transform of f, defined by

$$\hat{f}(\boldsymbol{p}) = \int_{\mathbb{R}^2} f(\mathrm{x})\, e^{-i\mathrm{x}\cdot\boldsymbol{p}}\, \mathrm{d}\mathrm{x}\,, \qquad f(\mathrm{x}) = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \hat{f}(\boldsymbol{p})\, e^{i\boldsymbol{p}\cdot\mathrm{x}}\, \mathrm{d}\boldsymbol{p}\,.$$

Ref: G. Beylkin, C. Kurcz, L. Monzón, *Fast algorithms for Helmholtz Green's functions*, Proc. R. Soc. A, **464**, (2008), pp. 3301-3326.

Key: PSF is critical for readily calculating a required Bloch Green's function.

Floquet-Bloch Theory

- Localize as $\varepsilon \to 0$ a steady-state spot for the GM system at $0 \in \Omega$. Extend periodically to $\mathbb{R}^2$.
- Linearize GM system around this steady-state solution. For $\varepsilon \to 0$, the eigenfunction Ψ corresponding to the long-range component u satisfies an elliptic PDE with coefficients that are spatially periodic on Λ.
- Thus, by the Floquet-Bloch theorem, we impose for ψ that

$$\psi(\mathbf{x} + \boldsymbol{l}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{l}}\,\psi(\mathbf{x})\,, \qquad \boldsymbol{l} \in \Lambda\,.$$

- **Formulate Boundary Operator on $\partial\Omega$:** Let L_i and L_{-i} be two parallel Bragg lines on opposite sides of $\partial\Omega$ for $i = 1, \ldots, L/2$, with $L = \{4, 6\}$. Let $\mathbf{x}_{i1} \in L_i$ and $\mathbf{x}_{i2} \in L_{-i}$ be any two opposing points on these Bragg lines. We define the boundary operator $\mathcal{P}_k\Psi$ by

$$\mathcal{P}_k\Psi \equiv \left\{ \Psi \,\middle|\, \begin{pmatrix} \Psi(\mathbf{x}_{i1}) \\ \partial_n\Psi(\mathbf{x}_{i1}) \end{pmatrix} = e^{-i\mathbf{k}\cdot\boldsymbol{l}_i} \begin{pmatrix} \Psi(\mathbf{x}_{i2}) \\ \partial_n\Psi(\mathbf{x}_{i2}) \end{pmatrix}, \right.$$
$$\left. \forall\, \mathbf{x}_{i1} \in L_i\,,\ \forall\, \mathbf{x}_{i2} \in L_{-i}\,,\ \boldsymbol{l}_i \in \Lambda\,,\ i = 1, \ldots, L/2 \right\}.$$

- The boundary operator $\mathcal{P}_0\Psi$ simply corresponds to periodic BC on $\partial\Omega$.

Key Results For Certain Green's Functions

There are two key Green's functions on Ω that play a central role:

Key 1: The source-neutral or periodic G-function is

$$\Delta G_{0p} = \frac{1}{|\Omega|} - \delta(\mathbf{x}), \quad \boldsymbol{x} \in \Omega; \qquad \mathcal{P}_0 G_{0p} = 0, \quad \mathbf{x} \in \partial\Omega,$$

$$G_{0p} \sim -\frac{1}{2\pi} \log|\mathbf{x}| + R_{0p} + o(1), \quad \text{as} \quad \mathbf{x} \to 0; \quad \int_\Omega G_{0p}\, d\mathbf{x} = 0.$$

Theorem (Chen-Oshita, 2007): Fix $|\Omega| = 1$. The regular part R_{0p} is minimized for a regular hexagonal lattice. Also, $\exists$ an explicit formula for R_{0p}.

Key 2: The Bloch Green's function for $\mathbf{k}/(2\pi) \in \Omega_B$ satisfies

$$\Delta G_{b0} = -\delta(\mathbf{x}), \qquad \mathbf{x} \in \Omega; \qquad \mathcal{P}_k G_{b0} = 0, \quad \mathbf{x} \in \partial\Omega,$$

$$G_{b0} \sim -\frac{1}{2\pi} \log|\mathbf{x}| + R_{b0}(\mathbf{k}) + o(1), \quad \text{as} \quad \mathbf{x} \to 0.$$

Lemma [IRWW, 2014]: $R_{b0}(\mathbf{k})$ is real-valued, with $R_{b0}(\mathbf{k}) = \mathcal{O}(\left[\mathbf{k}^T Q \mathbf{k}\right]^{-1}) = \mathcal{O}(|\mathbf{k}|^{-2})$ as $|\mathbf{k}| \to 0$ for an orthogonal matrix Q.

Brief Sketch of Analysis: I

Steady-State Construction: Inner Region: Near $\mathbf{x} = 0 \in \Omega$, let $u = D\,U(\rho)$, $v = DV(\rho)$, $\rho \equiv \varepsilon^{-1}|\boldsymbol{x}|$. This gives the radially symmetric core problem

$$\Delta_\rho V - V + V^2/U = 0\,, \qquad \Delta_\rho U = -V^2\,, \quad \rho > 0$$
$$V \to 0\,, \quad U \sim -S \log\rho + \chi(S) + o(1)\,, \quad \text{as} \quad \rho \to \infty\,.$$

It is readily shown that $\chi(S) = \mathcal{O}(S^{1/2})$ as $S \to 0$.

Lemma [IRWW, 2014]: *For $S = S_0\nu^2 + S_1\nu^3 + \cdots$, where $\nu \equiv -1/\log\varepsilon \ll 1$, the asymptotics of the core solution for $S \to 0$ is*

$$V \sim \nu\left[\chi_0 w + \nu\left(\chi_1 w + S_0 V_{1p}\right) + \cdots\right)\,, \qquad \chi \sim \nu\left(\chi_0 + \nu\chi_1 + \cdots\right)\,,$$

where $w(\rho)$ is the ground state. Here V_{1p} is the unique solution to

$$L_0 V_{1p} \equiv \Delta_\rho V_{1p} - V_{1p} + 2wV_{1p} = w^2 U_{1p}\,; \quad V_{1p} \to 0\,, \ \text{as} \ \rho \to \infty\,,$$
$$\Delta_\rho U_{1p} = -w^2/b\,; \quad U_{1p} \to -\log\rho + o(1)\,, \ \text{as} \ \rho \to \infty\,,$$

where $b \equiv \int_0^\infty \rho w^2\, d\rho$. Finally, χ_0 and χ_1 are related to S_0 and S_1 by

$$\chi_0 = \sqrt{\frac{S_0}{b}}\,, \qquad \chi_1 = \frac{S_1}{2\chi_0 b} - \frac{S_0}{b}\int_0^\infty w V_{1p} \rho\, d\rho\,.$$

Brief Sketch of Analysis: II

Match to an outer solution for u. For $D = D_0/\nu$, S satisfies

$$\left[1 + \mu + 2\pi\nu R_{0p} + \mathcal{O}(\nu^2)\right] S = \nu\chi(S)\,, \qquad \mu \equiv \frac{2\pi D_0}{|\Omega|}\,. \qquad (\star)$$

To leading-order, $\lambda = 0$ when $\mu = 1$. Thus, we expand

$$\lambda = \nu\lambda_1 + \cdots\,, \qquad \text{for} \qquad \mu = 1 + \nu\mu_1 + \cdots\,.$$

From asymptotics of core problem and $(\star)$, we relate χ_1 to μ_1 by

$$\chi_1 = -\frac{\mu_1}{4b} - \frac{\pi R_{0p}}{2b} - \frac{1}{2b^2}\int_0^\infty w V_{1p}\rho\, d\rho\,.$$

Stability problem: expand $\Phi = w + \nu\Phi_1 + \cdots$ for $\mu = 1 + \nu\mu_1 + \cdots$. We get

$$\mathcal{L}\Phi_1 \equiv L_0\Phi_1 - w^2 \frac{\int_0^\infty w\Phi_1\rho\, d\rho}{\int_0^\infty w^2\rho\, d\rho} = \mathcal{F} + \lambda_1 w\,; \qquad \Phi_1 \to 0\,, \quad \text{as} \quad \rho \to \infty\,,$$

$$\mathcal{F} \equiv 2\pi R_{b0} w^2 + 2\chi_1 b w^2 + \frac{1}{2b} w^2 \int_0^\infty w V_{1p}\rho\, d\rho + w^2 U_{1p}\,.$$

Solvability Condition: Since $\mathcal{L}^\star\Psi^\star = 0$ with $\Psi^\star \equiv w + \rho w'/2$, we must have $\lambda_1 \int_0^\infty w\Psi^\star\rho\, d\rho + \int_0^\infty \mathcal{F}\Psi^*\rho\, d\rho = 0$. This, ultimately, relates λ_1 to μ_1.

GM: Main Result for Periodic Patterns

$$v_t = \varepsilon^2 \Delta v - v + v^2/u\,, \quad \tau u_t = D\Delta u - u + v^2\,; \qquad \text{(GM Model)}\,.$$

Principal Result [IRWW, 2014]: *For* $D \sim \frac{|\Omega|}{2\pi\nu}(1+\nu\mu_1)$, *the portion of the continuous spectrum satisfying* $|\lambda| \leq \mathcal{O}(\nu)$ *is*

$$\lambda = \nu\lambda_1 + \cdots\,, \quad \lambda_1 = \mu_1 - 4\pi R_{b0}(\mathbf{k}) + 2\pi R_{0p} - \frac{1}{b}\int_0^\infty \rho w V_{1p}\, d\rho\,.$$

Thus, a periodic arrangement of spots on Λ *is linearly stable when*

$$\mu_1 < \mu_1^\star \equiv 4\pi R_{b0}^\star - 2\pi R_{0p} + \frac{1}{b}\int_0^\infty w V_{1p}\rho\, d\rho\,, \quad R_{b0}^\star \equiv \min_{\mathbf{k}} R_{b0}(\mathbf{k})\,.$$

The optimal lattice arrangement maximizes

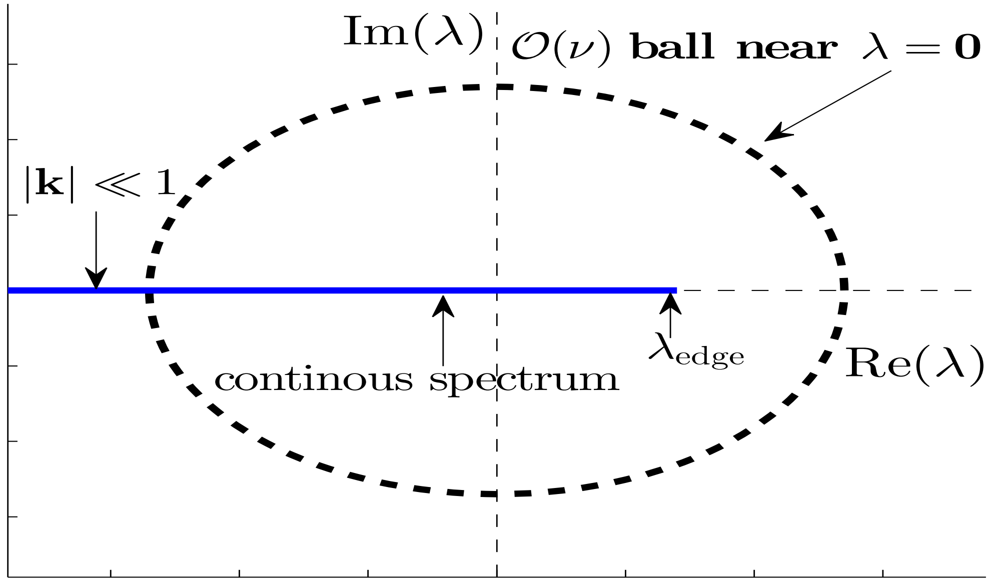
$$\mathcal{K}_{\text{gm}} \equiv 4\pi R_{b0}^\star - 2\pi R_{0p}$$

The stability threshold on the optimum lattice is

$$D_{\text{optim}} \sim \frac{|\Omega|}{2\pi\nu}\left[1 + \nu\left(\max_{\Lambda} \mathcal{K}_{\text{gm}} + \frac{1}{b}\int_0^\infty w V_{1p}\rho\, d\rho\right)\right]\,,$$

Numerical computations yield $b \approx 4.93$ *and* $\int_0^\infty w V_{1p}\rho\, d\rho \approx -0.945$.

Plot of the Spectrum Near Criticality



Remarks:

- Since $R_{b0}(\mathbf{k}) = \mathcal{O}(|\mathbf{k}|^{-2})$ as $|\mathbf{k}| \to 0$, long-wavelength perturbations are at a safe distance $\mathcal{O}(\nu/|\mathbf{k}|^2)$ along the negative real axis.
- **Recall:** $R_{b0}(\mathbf{k})$ is real-valued. Thus, the band is along real axis. Need only locate right-most edge of band.

A Formula for R_{b0} of Bloch G-Function

Challenge: Infinite series representation of G_{b0} in physical space has poor convergence properties. Challenging to efficiently compute $R_{b0}(\mathbf{k})$.

Ref: G. Beylkin, C. Kurcz, L. Monzón, *Fast algorithms for Helmholtz Green's functions*, Proc. R. Soc. A, **464**, (2008), pp. 3301-3326.

Introduce cut-off $\eta > 0$ representing "portion" of terms obtained from direct and reciprocal lattice. By using PSF between Λ and Λ^*, we get

$$R_{b0} = \sum_{\boldsymbol{d}\in\Lambda^*} \exp\left(-\frac{|2\pi\boldsymbol{d}-\boldsymbol{k}|^2}{4\eta^2}\right) \frac{1}{|2\pi\boldsymbol{d}-\boldsymbol{k}|^2} + \sum_{\substack{\boldsymbol{l}\in\Lambda \\ \boldsymbol{l}\neq 0}} e^{i\boldsymbol{k}\cdot\boldsymbol{l}} F_{\text{sing}}(\boldsymbol{l}) - \frac{\gamma}{4\pi} - \frac{\log\eta}{2\pi},$$

where γ is Euler's constant, $F_{\text{sing}}(\boldsymbol{l}) = E_1(|\boldsymbol{l}|^2\eta^2)/(4\pi)$, and $E_1(z)$ is exponential integral. Need only consider $\mathbf{k}/(2\pi) \in \Omega_B$.

Remark: Direct calculation using PSF and a key Hankel transform pair. Optimize η so as to get accuracy with as few terms as possible.

Numerics of R_{b0} of Bloch G-Function

Goal: Determine the lattice arrangement that maximizes $R_{b0}^{\star}$, where $R_{b0}^{\star} = \min_{\mathbf{k}\in\Omega_B} R_{b0}(\mathbf{k})$.

Key 1: For a given lattice, we must discretize the $\mathbf{k}$-space in the first Brillouin zone to compute the minimum of R_{b0} wrt $\mathbf{k}$.

Key 2: Must then sweep over all lattices for which $|\Omega| = 1$.

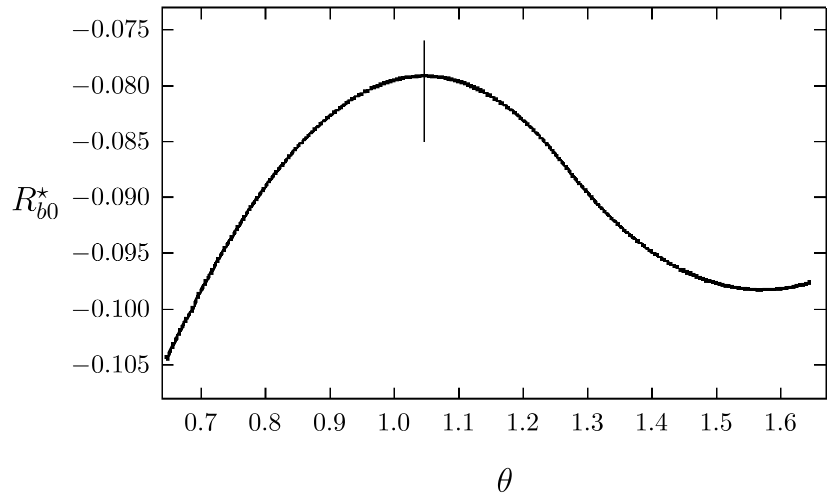
Sweeping over Ω: Numerical Computations of R_{b0}

Sweep I: $|\boldsymbol{l}_1| = |\boldsymbol{l}_2|$, with $|\Omega| = |\boldsymbol{l}_1||\boldsymbol{l}_2|\sin\theta = 1$. Let $\boldsymbol{l}_1 = (1/\sqrt{\sin(\theta)}, 0)$ and $\boldsymbol{l}_2 = (\cos(\theta)/\sqrt{\sin(\theta)}, \sqrt{\sin(\theta)})$ and sweep $0 < \theta < \pi/2$. **Regular Hexagon:** when $\theta = \pi/3$.

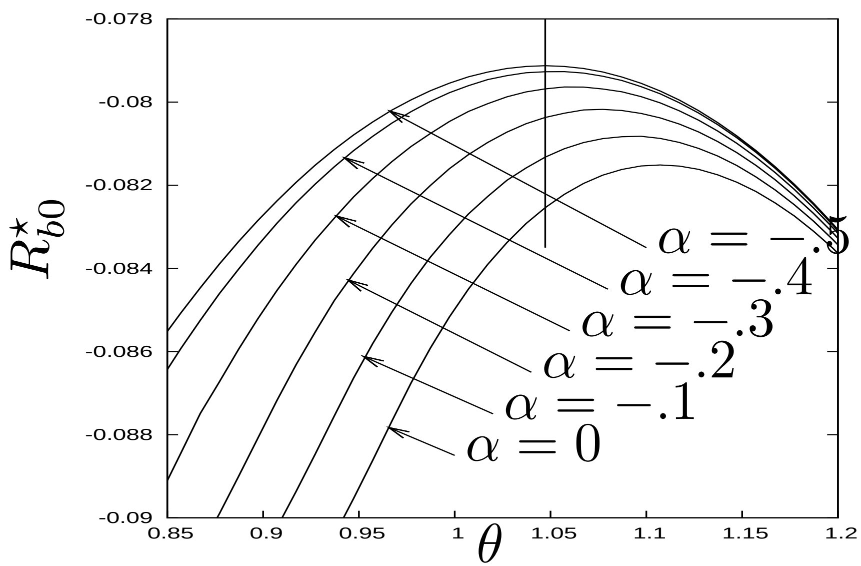
Sweep II: Let $\boldsymbol{l}_1 = (a, 0)$ and $\boldsymbol{l}_2 = (b, c)$, and introduce parameter α. Define $a = (\sin\theta)^{\alpha}$, $c = (\sin\theta)^{-\alpha}$ and $b = \cos\theta\ (\sin\theta)^{-\alpha-1}$. Then, $|\Omega| = 1$. Note: regular hexagon occurs only when $\alpha = -0.5$ (at $\theta = \pi/3$).

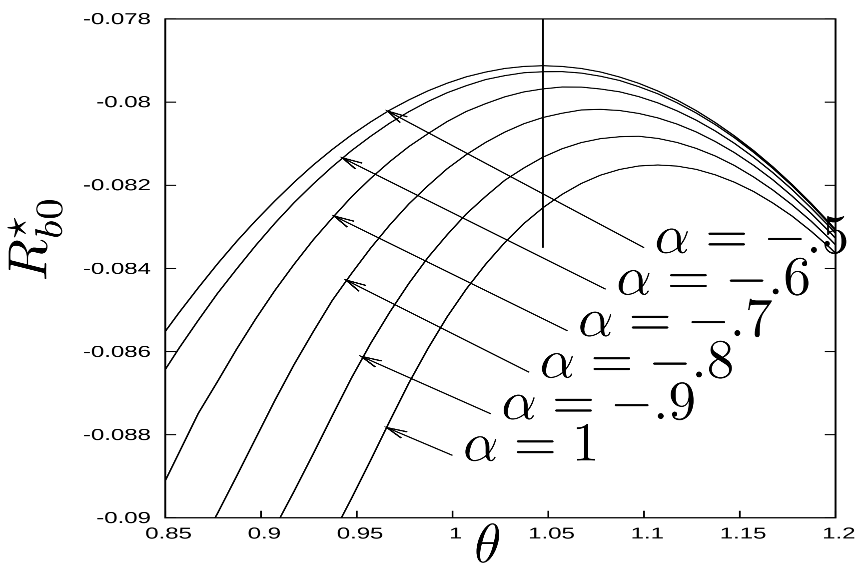
Numerical Computation of Optimal R_{b0}^*

Conjecture (based on numerics): The regular hexagon maximizes R_{b0}^*.



Sweep I: R_{b0}^* versus θ (above). **Sweep II:** $R_{b0}^{\star}$ versus θ for various α (below).





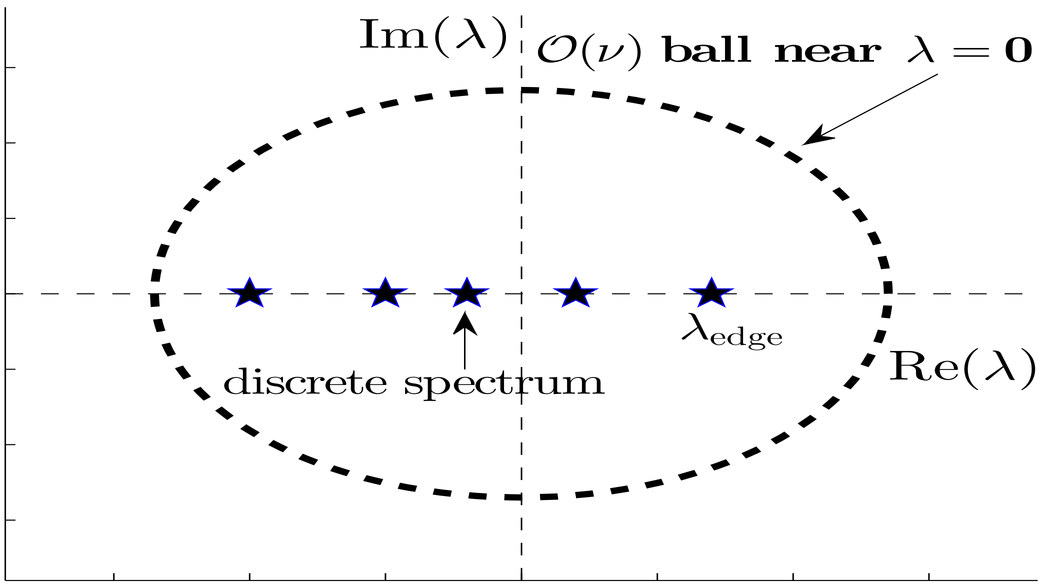
Finite Domain: Unfolding $\lambda = 0$:

Finite Domain Ω_f: Unfold the degenerate zero eigenvalue crossing for competition modes and calculate critical values μ_{1j} in

$$D_c \equiv \frac{D_{0c}}{\nu}\left(1 + \nu \mu_{1j}\right) + o(1)\,, \quad j = 1, \ldots, N-1\,; \qquad D_{0c} \equiv \frac{|\Omega_f|}{2\pi N}\,,$$

where individual modes cross through $\lambda = 0$.

- $\min_j \mu_{1j}$ to get stability threshold.
- **Remark:** possible degeneracies at higher order as well. **Ref: [Gomez-Ward-Wei, 2019]** to be submitted.



GM: Main Result for Finite Domain Ω_f

Principal Result [Gomez-Ward-Wei 2019]: *Let $N \geq 2$, and suppose $\boldsymbol{e} = (1.\ldots,1)^T$ is an eigenvector of Neumann Green's matrix $\mathcal{G}$. Then, for $D \sim \frac{|\Omega_f|}{2\pi N\nu}(1+\nu\mu_1)$, there are $N-1$ eigenvalues (counting multiplicity) in an $|\lambda| \leq \mathcal{O}(\nu)$ ball, which are given by:*

$$\lambda \sim \nu\lambda_{1i}\,, \quad \lambda_{1i} = \mu_1 - 4\pi\kappa_i + 2\pi\kappa_N - \frac{1}{b}\int_0^\infty \rho w V_{1p}\, d\rho\,, \quad i = 1,\ldots,N-1\,.$$

Here $\mathcal{G}\boldsymbol{e} = \kappa_N \boldsymbol{e}$ and $\mathcal{G}\mathbf{q}_i = \kappa_i \mathbf{q}_i$, with $\mathbf{q}_i^T \boldsymbol{e} = 0$ for $i = 1,\ldots,N-1$. Also, $\mathcal{G}_{ii} = R_i$, and $\mathcal{G}_{ij} = G_{ij}$ for $i \neq j$, where the Neumann $G(\mathbf{x};\xi)$ satisfies

$$\Delta G = \frac{1}{|\Omega_f|} - \delta(\mathbf{x}-\xi)\,, \quad \boldsymbol{x} \in \Omega_f\,; \qquad \partial_n G = 0\,, \quad \mathbf{x} \in \partial\Omega_f\,,$$

$$G \sim -\frac{1}{2\pi}\log|\mathbf{x}-\xi| + R(\xi) + o(1)\,, \quad \text{as} \quad \mathbf{x} \to \xi\,; \quad \int_{\Omega_f} G\, d\mathbf{x} = 0\,.$$

Remarks:

- **Correspondence to periodic problem:** $R_{0p} \to \kappa_N$ and $R_{b0}(\mathbf{k}) \to \kappa_i$.
- **Open Issue:** Establish the correspondence when $N \to \infty$.

Refined Competition Threshold

The competition instability threshold for $\nu = -1/\log \varepsilon \ll 1$ is

$$D_c \sim \frac{D_{0c}}{\nu}\left(1 + \nu \mu_{1c}\right), \qquad D_{0c} \equiv \frac{|\Omega_f|}{2\pi N},$$

where

$$\mu_{1c} \equiv -2\pi\kappa_N + 4\pi \min_{j\in\{1,\ldots,N-1\}} \kappa_j + \frac{1}{b}\int_0^\infty \rho w V_{1p}\, d\rho \,.$$

We have Re$(\lambda) < 0$ when $D < D_c$.

Qualitative: the competition stability threshold is determined by smallest matrix eigenvalue of the Neumann Green's matrix $\mathcal{G}$ in the $N-1$ dimensional subspace perpendicular to $(1, \ldots, 1)^T$.

For the disk, the Neumann G-matrix is readily calculated analytically in terms of the Neumann Green's function.

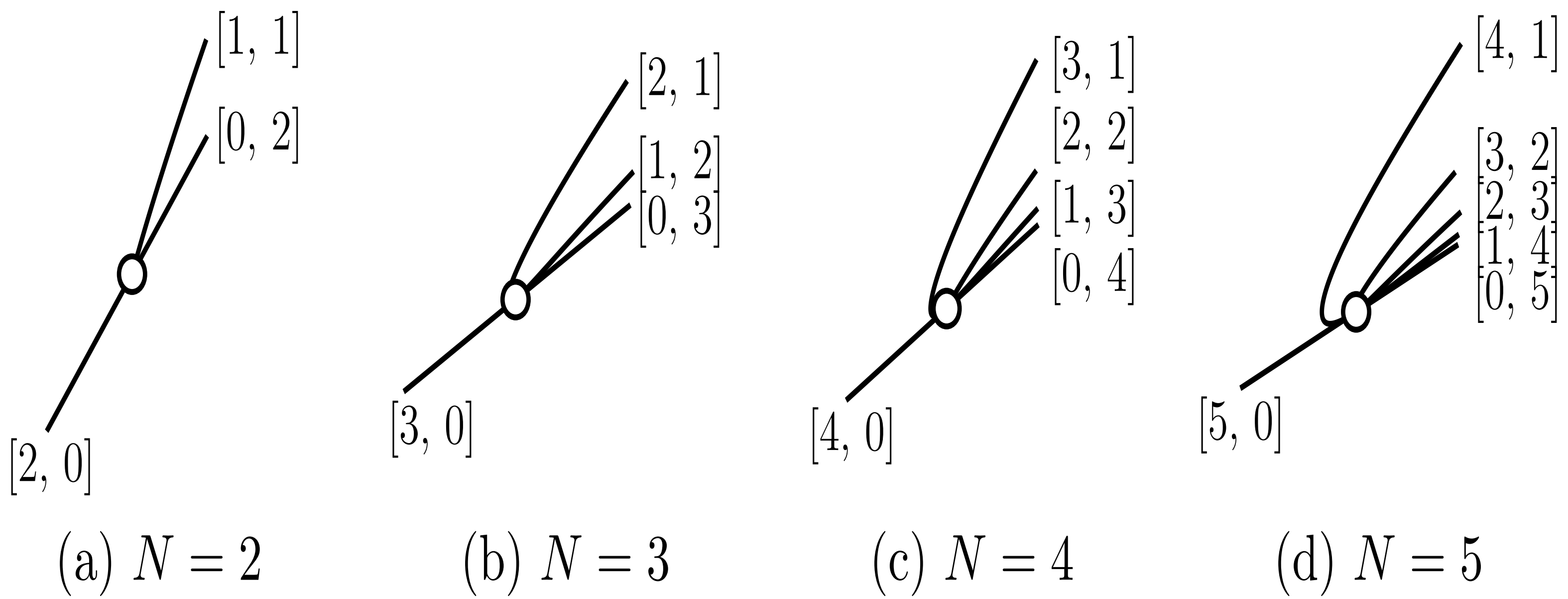
Questions:

- For the case where $\mathcal{G}\boldsymbol{e} = \kappa_N \boldsymbol{e}$ what does a a zero-eigenvalue crossing correspond to?
- What happens when $\boldsymbol{e}$ is not an eigenvector of $\mathcal{G}\boldsymbol{e}$?

Role of Symmetry Condition $\mathcal{G}_0 \mathbf{e} = \kappa_N \mathbf{e}$: I

NLEP stability theory is a leading-order-in-ν theory when $D = D_0/\nu$, based on a leading-order construction of the spot profile, i.e. the ground state w. Here $\lambda = 0$ crossing gives birth of *asymmetric* spot quasi-equilibria (i.e. spots of different amplitudes).

Local behavior of asymmetric branches in the leading-order theory as D crosses D_{0c}/ν:

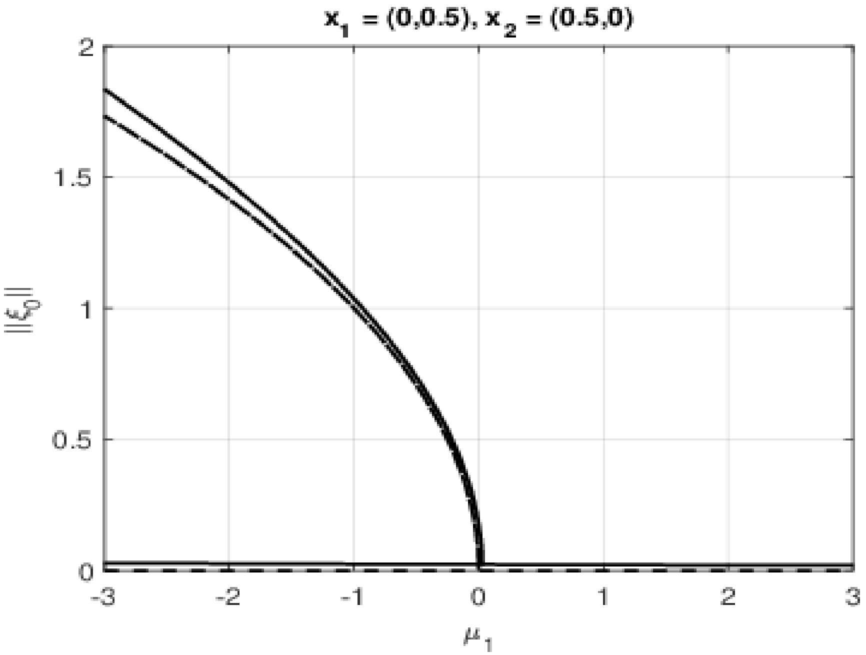


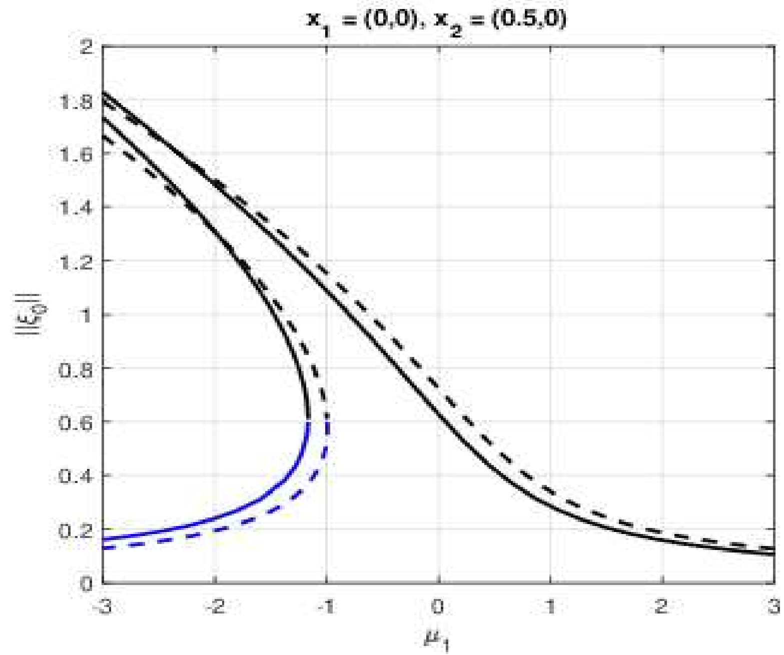
Question: Is branching "imperfection sensitive" to higher order terms in ν, i.e. is there a singular perturbation of the bifurcation?

Violation of Symmetry Condition: $\mathcal{G}\mathbf{e} \neq \kappa_N \mathbf{e}$

When e is not an eigenvector of $\mathcal{G}$, there is an imperfection sensitivity of steady-state solution branches near D_{0c}.

A local analysis near D_{0c} for a two-spot pattern yields:





Caption: Left: $\mathcal{G}\mathbf{e} = \kappa_N \mathbf{e}$ **Right:** $\mathcal{G}\mathbf{e} = \kappa_N \mathbf{e}$

Stability Theory: Open Questions

- For a given Ω, numerically identify both quasi-equilibrium and steady-state spot configurations for which the *symmetry condition* $\mathcal{G}_0 \mathbf{e} = \kappa_{01} \mathbf{e}$ holds. Go beyond ring patterns of spots. May need fast-multipole methods to compute $\mathcal{G}_0$.
- For any $N \geq 2$, analyze the local imperfection sensitivity of solution branches to the nonlinear algebraic system for $D = D_{0c}/\nu + O(1)$ when the symmetry condition fails to hold. **Ref:** Gomez-Ward-Wei (2019).
- Develop a weakly nonlinear theory for both competition instabilities and spot amplitude oscillations.
- Establish analytically for the periodic spot pattern that $R_{b0}^{\star}$ is maximized for a regular hexagon. Extend to Honeycomb-type lattices.
- For a periodic spot pattern, analyze the small eigenvalues of $\mathcal{O}(\varepsilon^2)$ (translation modes) in the linearization. What is now the optimal lattice? Need new Bloch-Green's function with dipole singularity. Do long-wavelengh peturbations set threshold? (Knobloch).

Recent References: Remarks

GM has been used only for illustration. Spot patterns arising in applications (urban crime model, plant root hair formation, Gray-Scott, Brusselator) and can be analyzed using similar methodologies.

<u>**References:**</u> **Available at http://www.math.ubc.ca/∼ward**

- [TWW] J. Tzou, M. J. Ward, J. Wei, *Anomalous Scaling of Hopf Bifurcation Thresholds for the Stability of Localized Spot Patterns for Reaction-Diffusion Systems in 2-D*, SIADS, **17**(1), (2018), pp. 982-1022.
- [IRWW, 2014] Iron, Rumsey, Ward, Wei, *Logarithmic expansions and the Stability of Periodic Patterns of Localized Spots for RD Systems in* $\mathbb{R}^2$, J. Non. Sci., **24**(5), (2014), pp. 857–912.
- [W] M. J. Ward, *Spots, Traps, and Patches: Asymptotic Analysis of Localized Solutions to some Linear and Nonlinear Diffusive Processes*, Nonlinearity, **31**(8), (2018), R189 (53 pages). (invited review article).

Part II: Brusselator on the Sphere

$$v_t = \varepsilon^2 \Delta_s v + \varepsilon^2 \mathrm{E} - v + f v^2 u \,, \qquad \tau u_t = \Delta_s u + \frac{1}{\varepsilon^2}(v - v^2 u) \,.$$

Quasi-equilibrium patterns: Construct quasi-equilibrium localized spot patterns for $\varepsilon \to 0$ using SLPT.

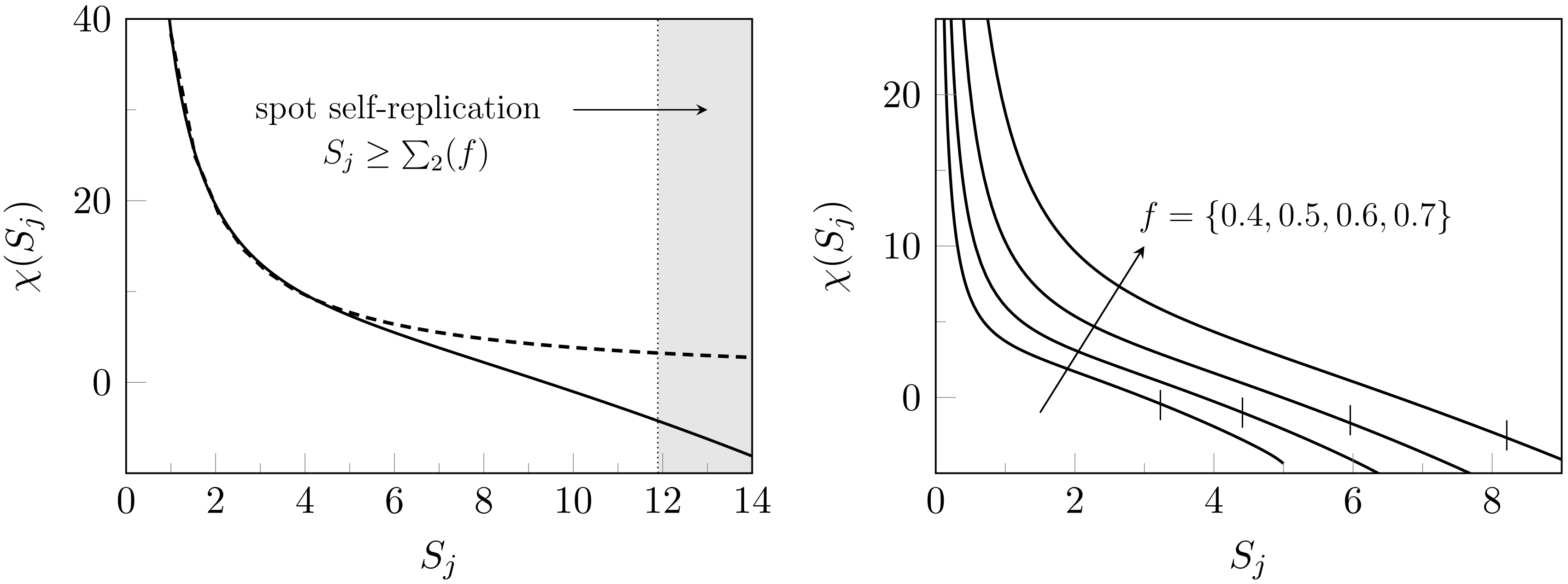
Core Problem: Consider a collection of N spots centered at $\mathbf{x}_j \,,\ j = 1, \ldots, N$. On the local-in-$\varepsilon$-tangent-plane at $\mathbf{x}_j$, we have the core problem:

$$\Delta_\rho V_{j0} - V_{j0} + f V_{j0}^2 U_{j0} = 0 \,, \qquad \Delta_\rho U_{j0} + V_{j0} - V_{j0}^2 U_{j0} = 0 \,,$$
$$V_{j0} \to 0 \,, \quad U_{j0} \sim S_j \log \rho + \chi + o(1) \quad \text{as } \rho \to \infty.$$

Here $\chi = \chi(S_j; f)$ must be computed numerically.

Peanut-Splitting Instability: Numerical computations of a 1-D eigenvalue problem show that for $S_j > \Sigma_2(f)$, the j-th spot is linearly unstable on an $\mathcal{O}(1)$ time-scale to peanut-splitting. This is the trigger of a nonlinear spot self-replication event.

Part II: Quasi-Equilibrium Patterns I



Caption: Left: χ versus S_j for $f = 0.3$ (heavy solid), compared with asymptotics. Right: χ versus S_j for $f = 0.4$, $f = 0.5$, $f = 0.6$, and $f = 0.7$, showing spot self-replication threshold $S_j = \Sigma_2(f)$ as thin vertical line.

Quasi-Equilibrium Patterns II

Outer Approximation: The leading-order inhibitor field satisfies

$$\Delta_S u = -\mathrm{E} + 2\pi \sum_{i=1}^{N} S_i \delta(\mathbf{x} - \mathbf{x}_i)\,, \qquad \sum_{i=1}^{N} S_i = 2\mathrm{E}\,,$$

$$u \sim S_j \log|\mathbf{x} - \mathbf{x}_j| - S_j \log\varepsilon + \chi(S_j)\,, \quad \text{as} \quad \mathbf{x} \to \mathbf{x}_j\,.$$

In terms of the well-known source-neutral Green's function G,

$$u = -2\pi \sum_{i=1}^{N} S_i G(\mathbf{x}; \mathbf{x}_i) + \overline{v} = \sum_{i=1}^{N} S_i L_i(\mathbf{x}) - (2\log 2 - 1)\mathrm{E} + \bar{u}\,.$$

Asymptotic Matching: gives a nonlinear algebraic system (NAS) for the S_j:

$$S_j + \nu\chi(S_j; f) - \nu \sum_{\substack{i=1 \\ i\neq j}}^{N} S_i L_{ij} = \bar{u}_c\,, \quad j = 1, \ldots, N\,; \qquad \sum_{i=1}^{N} S_i = 2\mathrm{E}\,,$$

where ν, L_{ij}, and $\bar{u}_c$ are defined by

$$\nu \equiv -1/\log\varepsilon\,, \qquad L_{ij} = \log|\mathbf{x}_i - \mathbf{x}_j|\,, \qquad \bar{u} \equiv \frac{\bar{u}_c}{\nu} + (2\log 2 - 1)\mathrm{E}\,.$$

NLEP Theory: Competition Instabilities

Consider $\mathrm{E} = \mathcal{O}(\sqrt{\nu})$, and spot patterns for which $S_j = \mathcal{O}(\sqrt{\nu})\ \forall j$.

To leading-order in ν, the stability of these patterns is characterized in terms of the discrete eigenvalues of a class of NLEP of the form

$$L_0\Phi - \beta(\lambda) w^2 \frac{\int_0^\infty w\Phi\rho\, d\rho}{\int_0^\infty w^2\rho\, d\rho} = \lambda\Phi\,, \qquad \Phi \to 0 \quad \text{as} \quad \rho \to \infty\,;$$

where $\Delta_\rho w - w + w^2 = 0$ and $L_0\Phi \equiv \Delta\Phi - \Phi + 2w\Phi$, and

$$\beta(\lambda) = \frac{a_1 + b_1\lambda + c_1\lambda^2}{a_2 + b_2\lambda + c_2\lambda^2}\,, \qquad \text{bi-quadratic}$$

- This NLEP is independent of the spot locations.
- Extend NLEP theory to allow for a bilinear $\beta(\lambda)$.

Main Result: For $\mathrm{E} < \frac{N\sqrt{\nu d_0}}{2}$ where $d_0 \equiv b(1-f)/f^2$ and $b \approx 4.934$, there are no positive real eigenvalues and hence no competition instabilities.

Scaling Law: The number N of spots with a common S_j that are stable is

$$\frac{2\mathrm{E}}{\Sigma_2(f)} < N < \frac{2\mathrm{E}}{\sqrt{\nu}} \frac{f}{\sqrt{b(1-f)}}\,, \qquad b \approx 4.934\,.$$

Brusselator: Slow Spot Dynamics I

A higher-order calculation yields the following reduced DAE system:

Principal Result: *For $\varepsilon \to 0$, and provided that the q.e. pattern is stable on an $\mathcal{O}(1)$ time-scale, the dynamics of a collection of N spots satisfies the DAE system for $S_1, \ldots, S_N$ and $\mathbf{x}_1, \ldots, \mathbf{x}_N$ on long time-scale $\varepsilon^2 t$:*

$$\frac{d\mathbf{x_j}}{dt} = \frac{2\varepsilon^2}{\mathcal{A}_j} (\mathrm{I} - \mathcal{Q}_j) \sum_{\substack{i=1 \\ i \neq j}}^{N} \frac{S_i \mathbf{x}_i}{|\mathbf{x}_i - \mathbf{x}_j|^2} \,, \qquad \mathcal{Q}_j \equiv \mathbf{x}_j \mathbf{x}_j^T \,, \qquad j = 1, \ldots, N \,,$$

coupled to the nonlinear algebraic constraint (NAS)

$$\mathcal{N}(\mathbf{S}) \equiv \Big[\mathrm{I} - \nu (\mathrm{I} - \mathcal{E}_0) \mathcal{G} \Big] \mathbf{S} + \nu (\mathrm{I} - \mathcal{E}_0) \chi(\mathbf{S}; f) - \frac{2\mathrm{E}}{N} \mathbf{e} = \mathbf{0} \,.$$

Here $\mathcal{A}_j = \mathcal{A}(S_j; f) < 0$ is defined via an integral.
Also I is the identity matrix, $(\mathbf{S})_i = S_i$, $(\mathcal{E}_0)_{ij} = \frac{1}{N}$, $(\chi(\mathbf{S}; f))_i = \chi(S_i)$, $(\mathbf{e})_i = 1$, $\nu = -1/\log \varepsilon$, and the Green's matrix $\mathcal{G}$ is

$$(\mathcal{G})_{ij} = \log |\mathbf{x}_i - \mathbf{x}_j| \,, \quad i \neq j \,; \qquad (\mathcal{G})_{ii} = 0 \,.$$

Slow Spot Dynamics: Basics I

Derivation: Higher-order matching between core solution and inhibitor field. Inhibitor field represented in terms of source-neutral Green's function on the sphere. Key Difficulty: Must go beyond simply projecting the local core solution centered at $\mathbf{x}_j$ onto the tangent-plane to the sphere. Then, apply solvability condition.

Property I: $\mathrm{I} - \mathcal{Q}_j$ projects onto the sphere, i.e. if $\mathbf{x}_j(0)$ satisfies $|\mathbf{x}_j(0)| = 1$, then $|\mathbf{x}_j(\sigma)| = 1\,,\ \forall \sigma > 0$.

Property 2: Equilibria of the dynamics are invariant under multiplication by an orthogonal matrix $\mathcal{R}$.

Property 3: If the pattern $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ of spots are such that $\mathcal{G}\mathbf{e} = \kappa_1 \mathbf{e}$ then, the pattern has a common source strength, i.e.

$$S_1 =, \ldots, S_N = S_c \equiv \frac{2\mathrm{E}}{N}\,.$$

This property holds for spots equi-distantly placed on a ring, for all platonic solids, any two-spot pattern, twisted cuboids, the icosahedron.

Slow Spot Dynamics: Basics II

Property 4: If we set $S_j = S_c$ for all j in the dynamics, then stable equilibria of the dynamics are local minima of the discrete logarithmic energy

$$\mathcal{H}_L(x_1, \ldots, x_N) \equiv -\sum_{i=1}^{N} \sum_{j>i}^{N} \log |\mathbf{x}_i - \mathbf{x}_j| \,, \qquad |x_j| = 1 \,, \quad j = 1, \ldots, N \,.$$

Elliptic fekete point sets are global minimizers of $\mathcal{H}_L$ **Proof:** Use Lagrange multipliers and project to the sphere.

Property 5: To leading order in ν, the NAS has solutions $S_j = S_c + \mathcal{O}(\nu)$ for all j. Thus, to leading-order in ν, elliptic Fekete point sets are stable equilibria of DAE dynamics.

Recall: For $i = 1, \ldots, N$, that Eulerian point vortex dynamics satisfy

$$\mathbf{x}_j' = \frac{1}{2\pi} \sum_{\substack{i=1 \\ i \neq j}}^{N} \Gamma_i \frac{\mathbf{x}_i \times \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^2} \,, \qquad j = 1, \ldots, N \,; \qquad \sum_{i=1}^{N} \Gamma_i = 0 \,.$$

Slow Spot Dynamics: Small N Results I

Main Goal: For fixed N, we start with 50 random initial locations $\mathbf{x}_i(0)$, for $i = 1, \ldots, N$, representing a collection of spots on the sphere. Our goal is to characterize equilibrium states of DAE with large basin of attractions.

Small N Equilibria: $N = 2, .., 8$ (All are Elliptic Fekete Point Sets)

- **N=2:** two antipodal spots ($S_1 = S_2$)
  Lemma (2-Spot Dynamics): Let $\mathbf{x}_2^T \mathbf{x}_1 = \cos \gamma_{1,2}$. Then, $S_1 = S_2 = \mathrm{E}$, and the solution of the DAE is

$$\cos\left(\gamma_{1,2}/2\right) = \cos\left(\gamma_{1,2}(0)/2\right) e^{-\mathrm{E}\varepsilon^2 t/|\mathcal{A}(\mathrm{E})|} \,,$$

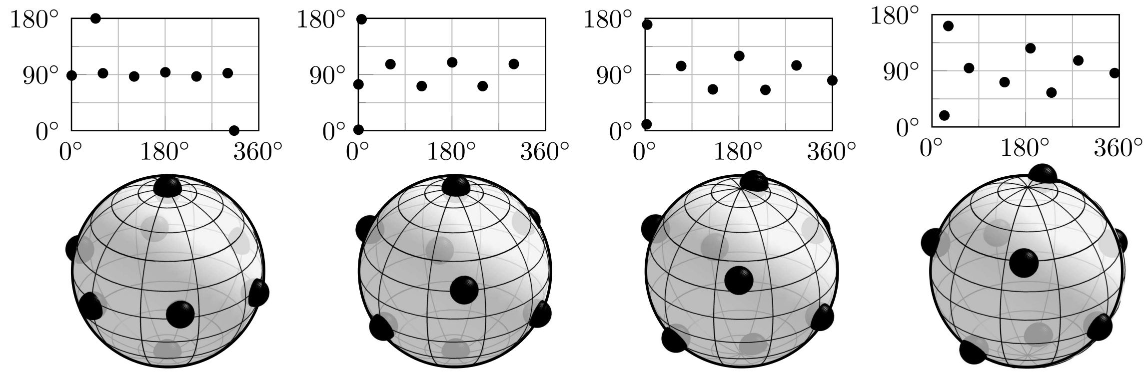
  so that $\gamma_{1,2} \to \pi$ as $\sigma \to \infty$ for any $\gamma_{1,2}(0)$.
- **N=3:** Three equally-spaced spots on a equator ($S_1 = S_2 = S_3$).
- **N=4:** Spots at vertices of a tetrahedron ($S_j = S_c$ for $j = 1, \ldots, 4$).
- **N=5,6,7:** Two antipodal spots, with $N - 2$ spots equally-spaced on the mid-plane. Two source strengths S_p and S_c.
- **N=8:** “Twisted Cuboid”. ($S_j = S_c \; \forall j$)

Slow Spot Dynamics: Small N Results II

Define: Ring pattern: consists of N particles on an equator. $(N-2)+2$ pattern: consists of $N-2$ particles on an equator with two polar spots.

Remarks (Numerics):

- Ring patterns are unstable for $N > 3$ (orbitally stable if $N \leq 3$)
- $(N-2)+2$ patterns are orbitally stable for $N = 4, 5, 6, 7$, but unstable if $N \geq 8$.

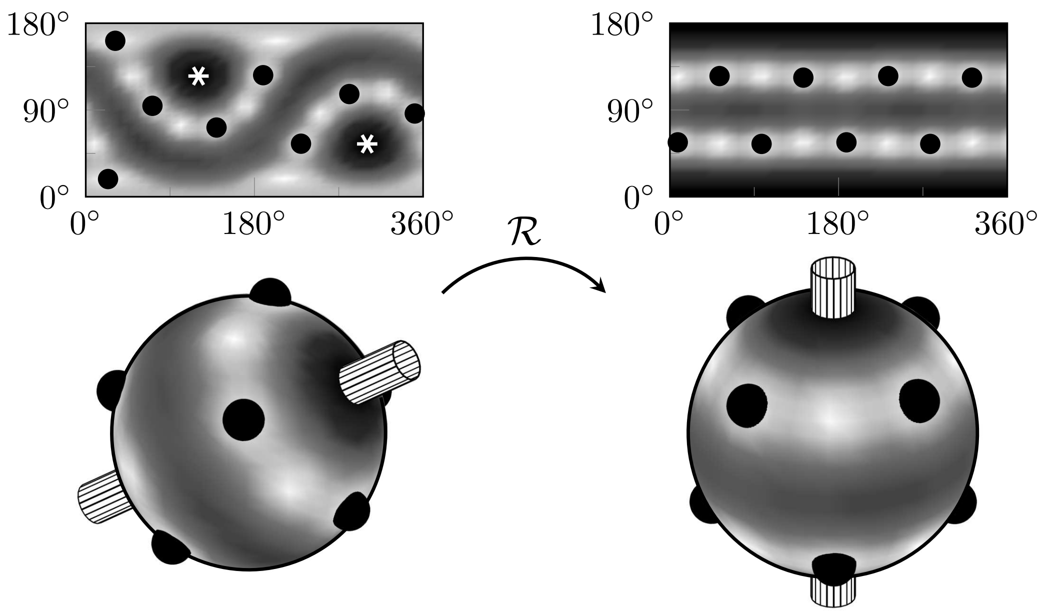


(a) $\sigma = 2$ (b) $\sigma = 3.5$ (c) $\sigma = 7$ (d) $\sigma = 25$

Caption: For $f = 0.5$, $\mathrm{E} = 16$, and $\varepsilon = 0.02$. Eight spots in an $(N-2)+2$ pattern undergo a 1% random perturbation at time $t = 0$. The initial $(N-2)+2$ pattern is unstable. Plot at different $\sigma = \varepsilon^2 t$.

Remark: Patterns become more difficult to visualize at larger N.

Twisted Cuboid Equilibrium: $N = 8$



Caption: Left: The shading on the sphere and top (ϕ, θ) plane indicate with two asterisks a better location to place the polar axis of the sphere (marked by a cylinder). **Right:** After an orthogonal transformation, $\mathcal{R}$.

N=8 Equilibria Pattern is a 45° twisted cuboid consisting of two parallel planes, each with 4 equally-spaced spots. The spots on the two planes are 45° phase-shifted. The ratio of the distance between neighboring spots on a ring to the perpendicular distance between the planes is 0.967. This yields the plane latitudes $\theta \approx 55.6^\circ$ and $\theta \approx 124.4^\circ$. ($S_j = S_c$ for $j = 1, \ldots, 8$). This is the elliptic Fekete point pattern for 8 particles.

Slow Spot Dynamics: Elliptic Fekete Points

Numerical Observation: Elliptic Fekete points lead to a $\mathcal{G}$ matrix for which $\mathbf{e}$ is nearly an eigenvector (see Table). **Q:** Can this numerical finding be “justified” theoretically, i.e. is there an asymptotic equi-partition of the discrete logarithmic energy for large N?

Number of points N	$\|\|\xi - \mathbf{e}\|\|_2$
8	$6.0301e-16$
10	0.0216
20	0.0050
50	0.0029
100	0.0029
120	0.0015
130	0.0027

Caption: The distance $\|\| \ldots \|\|_2$ between the principal eigenvector ξ of $\mathcal{G}$ and $\mathbf{e}$, both normalized, for different elliptic Fekete point configurations. For $N = 8$, where the elliptic Fekete point set is a rotated cuboid, the first row yields to machine precision that $\mathbf{e}$ is an eigenvector of $\mathcal{G}$. For comparison, a random distribution of 100 points on the sphere has a norm difference of 0.2512.

Broader: Narrow Capture Problems

Similar problems with logarithmic interactions occur in other 2-D such as for narrow capture problems involving a Brownian particle on the surface Ω of the unit sphere in the presence of localized traps:

$$\Delta_s u + \lambda u = 0 \,, \quad \mathbf{x} \in \Omega \backslash \Omega_p \,, \quad \Omega_p \equiv \cup_{i=1}^{N} \Omega_{\varepsilon_i} \,,$$

where Ω_{ε_i} is a “disk” of radius ε centered at $\mathbf{x}_i \in \Omega$. Then,

$$\lambda_0(\varepsilon) \sim \frac{\mu N}{2} + \mu^2 \left[-\frac{N^2}{4} \left(2\log 2 - 1\right) - \mathcal{H}_L(\mathbf{x}_1, \ldots, \mathbf{x}_N) \right] + \mathcal{O}(\mu^3) \,,$$

where with $\mu \equiv -1/\log \varepsilon$ *and* $\mathcal{H}(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ *is the discrete logarithmic energy*

$$\mathcal{H}(\mathbf{x}_1, \ldots, \mathbf{x}_N) \equiv -\sum_{i=1}^{N} \sum_{j>i}^{N} \log |x_i - x_j| \,.$$

Key Point: $\lambda_0(\varepsilon)$ is maximized at the elliptic Fekete points.

Reference: [CSW] Coombs, Straube, Ward, SIAM 2009.

Open Questions and Extensions

- Use symmetry groups, and point matching algorithms from CS to classify all equilibria of DAE system for larger N. What is basin of attraction of equilibria? Stability of Equilibria of DAE system?
- Explore relation between elliptic Fekete points and equilibria of DAE system for large N. When is $\mathbf{e}$ an eigenvector of the Green's matrix $\mathcal{G}$?
- Our analysis is based (largely) on formal asymptotics. Rigorous proof?

Extensions of the Model and Methodology:

- Formulate and analyze coupled bulk-surface RD systems.
- Analyze localized spot patterns for Brusselator on manifolds. The key here is to compute the Neumann G-function on a closed manifold: $\Delta_s G = |\Omega|^{-1} - \delta(x - x_0)$. Hybrid asymptotic numerical description of pattern formation. (Movie)

References:

- **[RRW] Rozada, Ruuth, Ward; The Stability of Localized Spot Patterns for the Brusselator on the Sphere**, SIADS **13**(1), (2014), pp. 564–627.
- **[TW] Trinh, Ward; Dynamics of Localized Spot Patterns for RD Systems on the Sphere**, Nonlinearity, **29**(3), (2016), pp. 766–806.