Refined Linear Stability Theory for 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

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

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

Key: Since $\epsilon \ll 1$, 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:** $\nu = -1/\log\epsilon$ is expansion parameter.
  - (II) Spot interactions via Green's functions and Green's matrices
  - (III) Optimization of stability thresholds yield new (discrete) variational problems.

RD Modeling with Localized Spots: I

- biological morphogenesis (Meinhardt 1984–), gene expresssion time delays (Gaffney 2005–2010): (GM Model and its variants, delayed reaction-kinetics, etc) Analysis: Wei, Winter, MJW, Doelman, Kaper... 1998–.
- chemical instabilities and self-replicating spot patterns in FIS reaction (Swinney 1994, Pearson 1994). (Gray Scott Model) Analysis: Doelman, Kaper, Gardner, Nishiura, Wei, Winter, Kolokolnikov, MJW, 2000–2012...
- Plant root-hair formation driven by auxin gradient (Payne, Grierson 2009): (Schnakenberg-type model with spatially heterogeneous nonlinearity). Analysis: Brena-Medina, Champneys, Avitabile, MJW, 2014–
- Spatial distribution of urban crime with or without police intervention (based on UCLA Group, Bertozzi, Short,..2009–); (3-component RD system with chemotaxis): Analysis of Crime Hotspots: Berestycki, Pitcher, Kolokolnikov, Ward, Wei, Winter, Tse,...

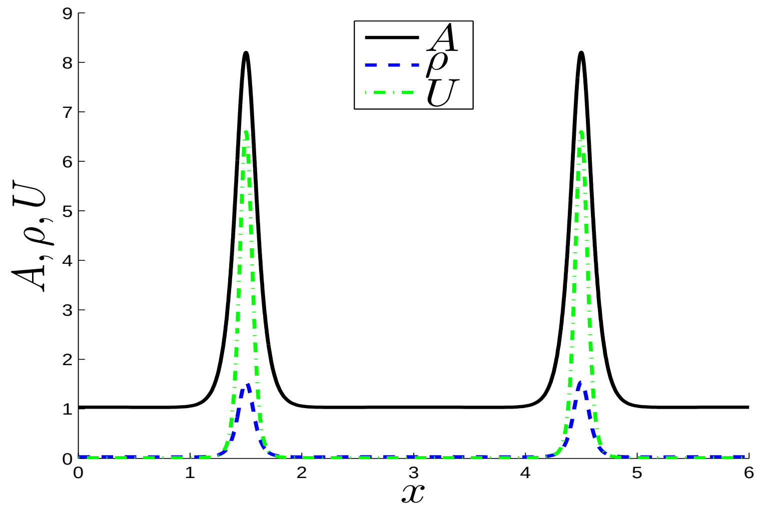
RD Modeling with Localized Spots: II

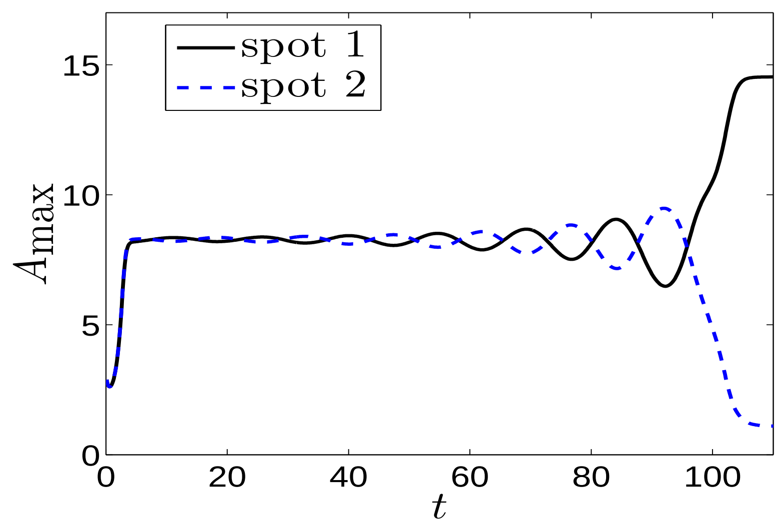
Three-component crime RD model with $A(\mathbf{x},t)$ is " attractiveness field" for burglarly, $P(\mathbf{x},t)$ is criminal density, and $U(\mathbf{x},t)$ is police density:

$$A_t = \epsilon^2 \Delta A - A + PA + \alpha\,, \quad x \in \Omega\,;$$

$$P_t = D\nabla \cdot \left(\nabla P - \frac{2P}{A} \nabla A \right) - PA + \beta - U\,, \quad x \in \Omega\,.$$

$$\tau_u U_t = D\nabla \cdot \left(\nabla U - \frac{2U}{A} \nabla A \right)$$





Ref: Tse, MJW, to be submitted, SIADS, (2017). $\exists$ a range of parameters where police intervention simpy displaces crime between spatial regions.

Brusselator: Spot Patterns

(Backward) Focus for Today: Brusselator RD System in 2-D: Prigogine (1968)

Construct "Spot Patterns" for 2-D Brusselator (with no flux BC):

$$V_\sigma = \epsilon_0^2 \Delta V + E_f - (B+1)V + UV^2 \,, \quad U_\sigma = \mathcal{D}\Delta U + BV - UV^2 \,.$$

Asymptotic Limit: Assume large diffusivity ratio and small "fuel" E_f:

$$\epsilon_0 \ll 1 \,, \qquad D = \mathcal{O}(1) \,, \qquad E_f = \epsilon_0 E_0 E(\mathbf{x}) \,.$$

Introduce Rescaling: $V = E_0 v/\epsilon_0$, $U = \epsilon_0 B u/E_0$, and $\sigma = t/(B+1)$, to get:

Non-Dimensional Brusselator Model:

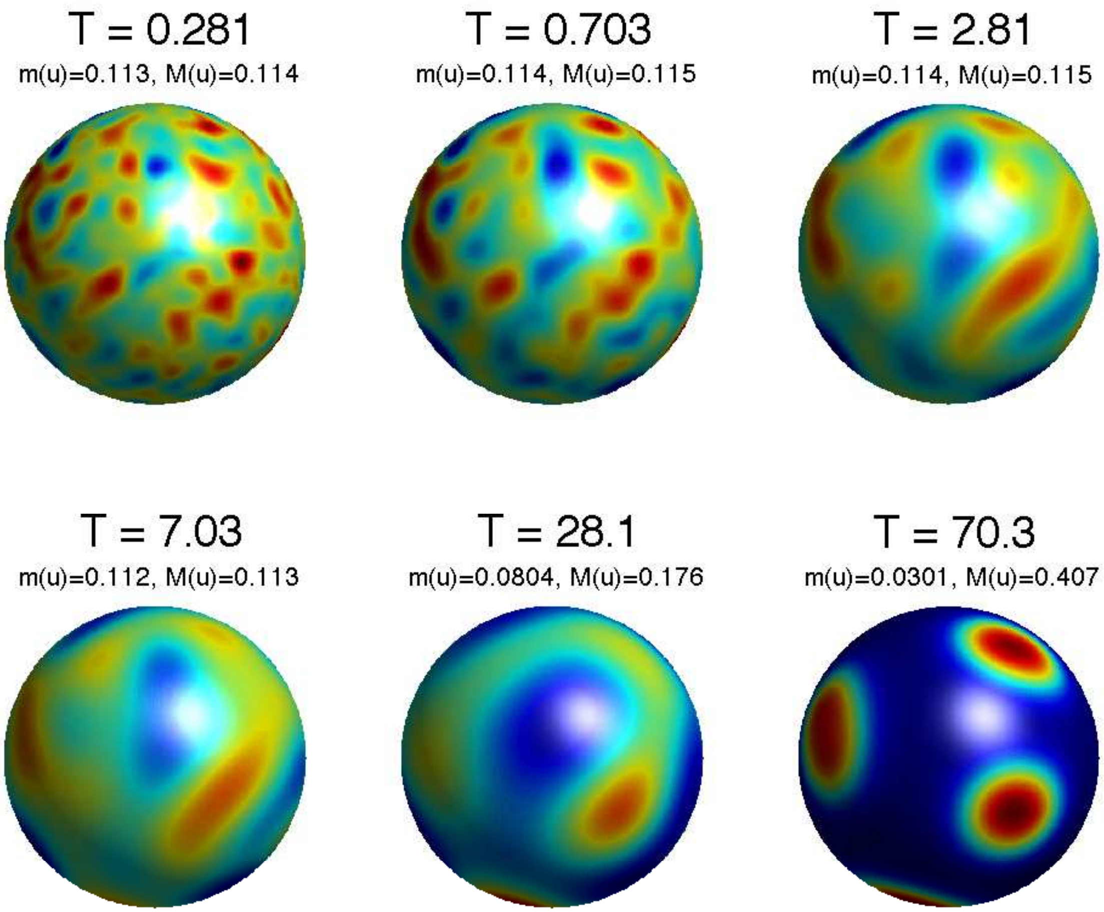
$$v_t = \epsilon^2 \Delta v + \epsilon^2 E - v + f u v^2 \,, \quad \tau u_t = D\Delta u + \frac{1}{\epsilon^2}\left(v - uv^2\right)$$

where $E = E(\mathbf{x}) = \mathcal{O}(1)$. The non-dimensional parameters are

$$f \equiv \frac{B}{B+1} < 1 \,, \quad \tau \equiv \frac{(B+1)^2}{E_0^2} \,, \quad D \equiv \frac{\mathcal{D}(B+1)}{E_0^2} \,, \quad \epsilon \equiv \frac{\epsilon_0}{\sqrt{B+1}} \,.$$

Brusselator: Spot Patterns (Visual)

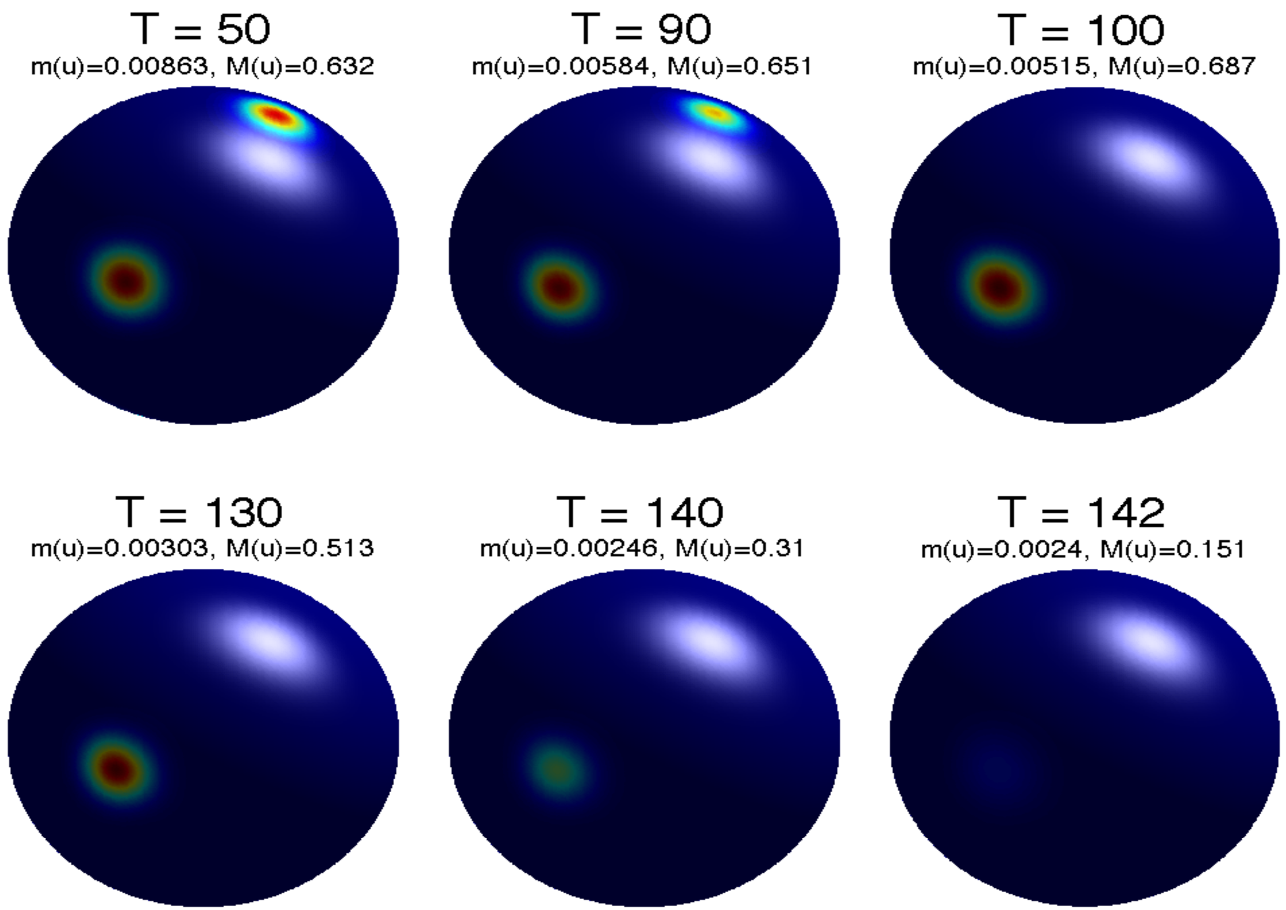
Full Numerics (S. Ruuth (SFU)): $f = 0.8$, $\epsilon = 0.075$, $D = 0.2$, $E = 4$, **and** $E_0 = 4$.
The initial data is a 2% **random perturbation from the spatially uniform state.**



- **[RRW]:** Very complicated transient dynamics due to the weakly nonlinear interaction of many unstable spherical harmonics. Linear and weakly nonlinear analysis not very useful in predicting the pattern.

Brusselator: Spot Instabilities I

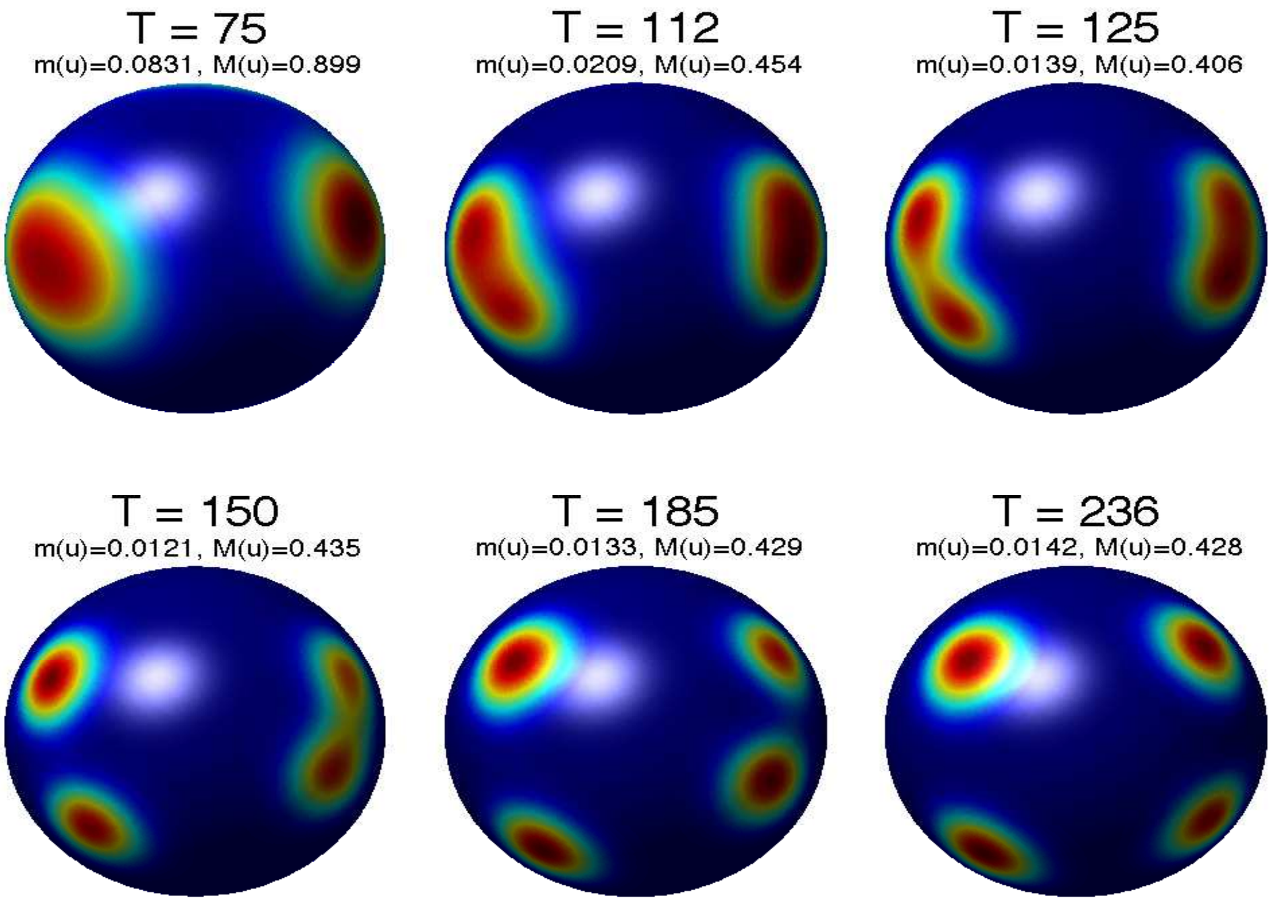
Competition instability as D crosses a threshold $D_c \gg 1$



Sign-alternating linear instability triggers nonlinear event which annihilates spots.

Brusselator: Spot Instabilities II

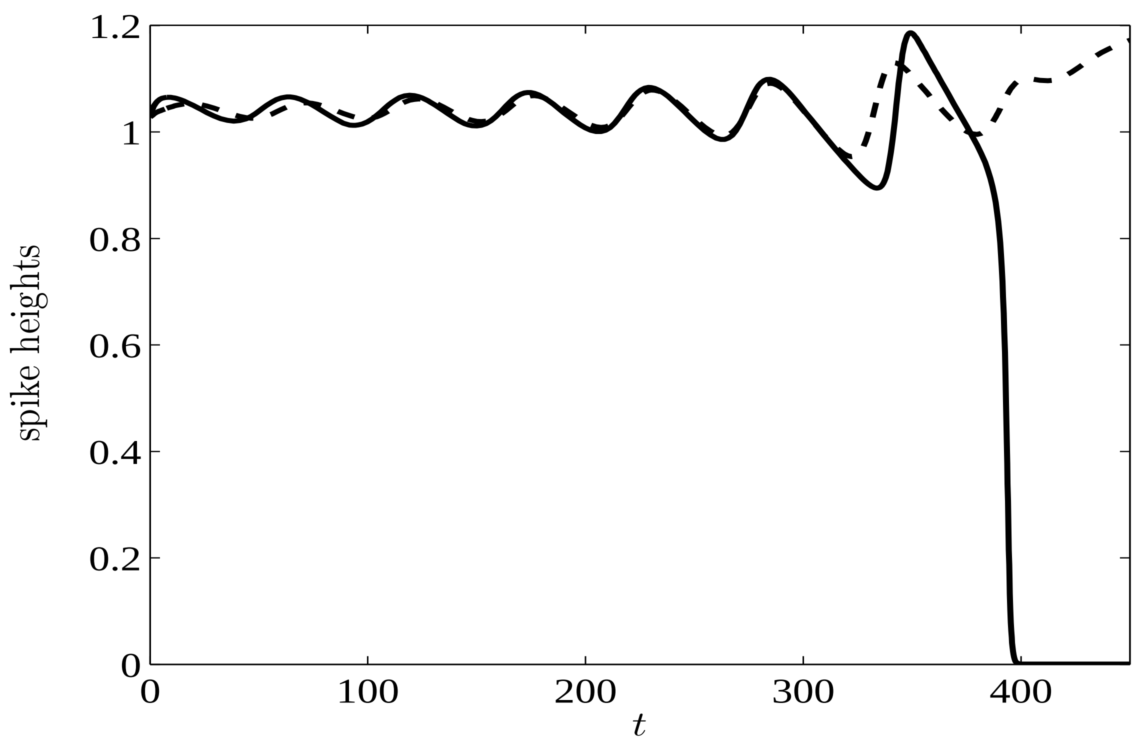
Spot Self-Replication: "Fuel" $E > E_c$ (Need $D = \mathcal{O}(1)$):



Peanut-splitting linear instability triggers nonlinear spot self-replication event.

Brusselator: Spot Instabilities III

Spot Amplitude Temporal Oscillations: as τ exceeds a threshold τ_H (2-spot ring pattern)



Oscillatory linear instability triggers a nonlinear spot collapse event.

Def: (Ring Pattern) Spots equidistantly spaced on a ring of radius r_0 concentric within the unit disk.

Spots: Outline of Theoretical Results

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

- **Self-replication instability** is only for $D = \mathcal{O}(1)$.
- **Competition Instability Threshold in 2-D Bounded Domains:** Determine refined asymptotic prediction for the critical value $D_c = \mathcal{O}(\nu^{-1}) \gg 1$ of D for a competition instability threshold.
- **Anomalous Scaling of a HB threshold** for spot amplitude oscillations as τ exceeds a threshold τ_H, with $\tau_H \gg 1$, when $D < D_c$.
- **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.

References:

- [CTWW] Y. Chang, J. Tzou, MJW, J. Wei, *Refined Stability Thresholds... for the Brusselator..*, submitted, EJAM (2017).
- [RRW] I. Rozada, S. Ruuth, MJW, *The Stability of Localized Spot Patterns ... on the Sphere*, SIADS, **13**(1), (2014).
- [W] MJW, *Spots, Traps, and Patches:...* , (invited “survey” for Nonlinearity, under revision, (2017)).

Quasi-Equilibrium Spot Patterns

Fix $N > 1$ and a **spatial configuration** for the centers $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \Omega$ of the spots with $|\mathbf{x}_j - \mathbf{x}_k| = \mathcal{O}(1)$. Consider the regime $D = D_0/\nu$ with $\nu = -1/\log \epsilon$. For E constant, a Q.E. solution satisfying

$$\epsilon^2 \Delta v + \epsilon^2 E - v + f u^2 v = 0 \,, \qquad \frac{D_0}{\nu} \Delta u + \frac{1}{\epsilon^2} \left(v - u v^2 \right) = 0 \,,$$

with concentration as $\epsilon \to 0$ at $\mathbf{x}_j$ for $j = 1, \ldots, N$ is:

$$v_e \sim \epsilon^2 E + \sum_{j=1}^{N} \frac{1}{f U_0} w \left[\epsilon^{-1} |\mathbf{x} - \mathbf{x}_j| \right] \,,$$

$$u_e \sim U_0 - \frac{E|\Omega|}{N D_0} \sum_{j=1}^{N} G_0(\mathbf{x}; \mathbf{x}_j) + O(1) \,, \quad |\mathbf{x} - \mathbf{x}_j| = \mathcal{O}(1) \,, \; \forall j = 1, \ldots, N \,.$$

Here G_0 is the Neumann G-function ($\Delta G_0 = |\Omega|^{-1} - \delta(\mathbf{x} - \mathbf{x}_j)$) and

$$U_0 \equiv \frac{2\pi b (1 - f)}{f^2 N E |\Omega|} \,, \qquad b \equiv \int_0^\infty \rho w^2 \, d\rho \,,$$

where $w(\rho)$ is the radially symmetric ground-state solution (spot profile)

$$\Delta_\rho w - w + w^2 = 0 \,, \quad \rho > 0 \,; \quad w(0) > 0 \,, \quad w \to 0 \quad \text{as} \quad \rho \to \infty \,.$$

NLEP Problem for Localized Spots: I

Linear stability analysis: The v-linearization has the form:

$$v \sim v_e + \sum_{j=1}^{N} c_j \Phi_j \left[\epsilon^{-1}|\mathbf{x} - \mathbf{x}_j|\right] e^{\lambda t} \,.$$

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" $(c_1, \ldots, c_N)^T$:

. . . . and after a detailed asymptotic calculation . . . .

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

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

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 $\mathcal{G}_\lambda$:

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

NLEP Problem for Localized Spots: II

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

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

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

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

$$\beta_j = \frac{2(\lambda+1-f)}{(\lambda+1)\left[1+\frac{D_0\theta}{1+2\pi\nu\kappa_j}\right]-f}\,, \qquad \theta \equiv \frac{4\pi^2 N^2(1-f)^2 b}{f^2 E^2 |\Omega|^2}\,.$$

Here $D_0 \equiv D\nu$, and $b \equiv \int_0^\infty \rho w^2\, d\rho$.

Remark: κ_j is undefined at $\lambda=0$. Need a limit analysis as $\lambda\to 0$ (easy fix).

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 Problem

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

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

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

$$2\pi\nu\kappa_1 \sim \frac{\mu}{\tau\lambda}\,; \quad 2\pi\nu\kappa_j = \mathcal{O}(\nu)\,, \quad \text{for} \quad j = 2,\ldots,N\,; \quad \mu \equiv \frac{2\pi N D_0}{|\Omega|}\,.$$

- $\mathbf{c}_1 = \mathbf{e}$ is the “synchronous mode”
- $\mathbf{c}_j = \mathbf{q}_j$ for $j = 2,\ldots,N$ are the “competition modes”: $\mathbf{q}_j^T\mathbf{e} = 0$.

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

$$\beta_c \equiv \frac{2(\lambda + 1 - f)}{(\lambda+1)\,(1 + D_0\theta) - f}\,,$$

$$\beta_s \equiv \frac{2(\lambda + 1 - f)}{(\lambda+1)h(\tau\lambda) - f}\,, \quad \text{where} \quad h(\tau\lambda) \equiv 1 + \frac{D_0\theta\tau\lambda}{\tau\lambda + \mu}\,.$$

Leading Order Competition Threshold

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

Main Result:[RRW] *Let $N \geq 2$ 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 $D_{0c} = (1 - f)/\theta$, yielding*

$$D_{0c} \equiv \frac{|\Omega|^2 f^2 E^2}{4\pi^2 N^2 b(1-f)}, \quad \text{where} \quad b \equiv \int_0^\infty \rho w^2 \, d\rho \, .$$

The competition threshold is $D_c \sim D_{0c}/\nu$ to leading order in $\nu \equiv -1/\log \epsilon$.

Remarks:

- The leading-order threshold is independent of the spot configuration.
- Need to unfold this $N-1$ dimensional zero-eigenvalue crossing to determine refined thresholds on a bounded domain and for periodic patterns on a Bravais lattice (see below), i.e. we need the next term

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

HB for Synchronous Mode I

Consider the **conventional NLEP regime** $\tau\nu|\lambda|/D_0 \ll 1$. Rigorously:

Main Result:[RRW] *If $D_0 > D_{0c}$, there is a Hopf bifurcation value for τ. If $D_0 < D_{0c}$, then $\exists\ \tau_2$ (small) and τ_3 (large) for which Re$(\lambda) < 0$ when either $0 < \tau < \tau_2$ or $\tau > \tau_3$.*

Implication: No HB can occur on $D_0 < D_{0c}$ when τ is small or large. What about intermediate τ?.

Remarks:

- Irrelevant that a HB exists for τ for the synchronous mode on $D > D_{0c}$ since competitition modes are all unstable on $D > D_{0c}\ \forall\tau \geq 0$.
- Same conclusion for GM, GS, Schnakenberg models (Wei-Winter). Long-standing open problem in 2-D NLEP theory.
- **Technical:** Analysis for Brusselator has a biquadratic in λ multiplier rather than a bilinear multiplier (Wei-Winter).
- Since $\beta_s(0) = 2$ for $\tau = 0$ and $\forall D_0$, then Re$(\lambda) < 0$ when τ is sufficiently small. Since $\beta_s = \beta_s(\tau\lambda)$, no zero-eigenvalue crossings can occur. By continuity of eigenvalue paths need only look for HB points.

HB for Synchronous Mode II

The discrete λ of the conventional NLEP (synchronous) are roots of

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

Set $\lambda = i\lambda_I$ and put $g(i\lambda_I) = 0$. This yields:

New parameterization: $D_0 = D_0(\lambda_I)$ and $\tau = \tau(\lambda_I)$ for any HB point:

$$D_0 = \frac{z_R^2 + z_I^2}{\theta z_I}\,, \qquad \frac{\tau}{\mu} = \frac{z_I}{\lambda_I z_R}\,, \quad \text{where} \quad \mu \equiv \frac{2\pi D_0(\lambda_I)}{|\Omega|}\,.$$

Here we have

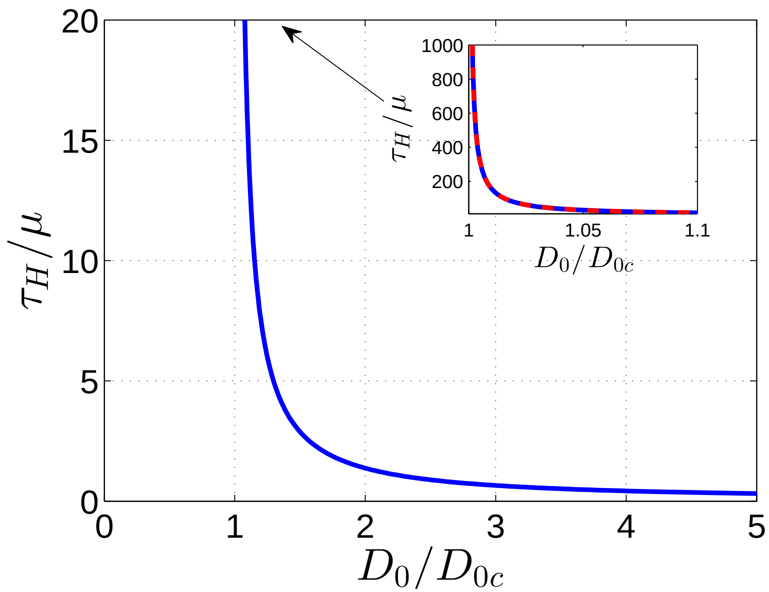
$$z_R \equiv \frac{k_I - \lambda_I k_R - \lambda_I f}{1+\lambda_I^2}\,, \qquad z_I \equiv \frac{k_R + \lambda_I k_I - \lambda_I^2 - (1-f)}{1+\lambda_I^2}\,,$$

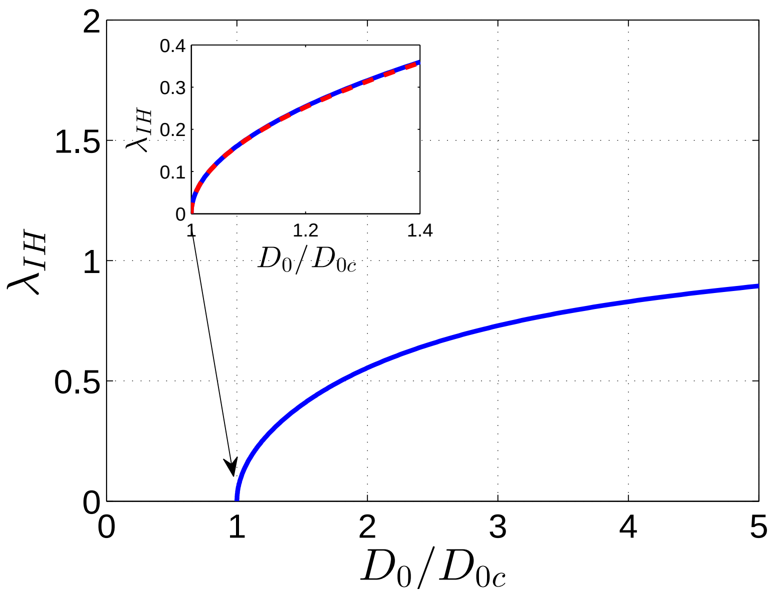
where with $\mathcal{F}(i\lambda_I) = \mathcal{F}_R(\lambda_I) + i\mathcal{F}_I(\lambda_I)$, we have

$$k_R \equiv 2(1-f)\mathcal{F}_R(\lambda_I) - 2\lambda_I \mathcal{F}_I(\lambda_I)\,, \quad k_I \equiv 2\lambda_I \mathcal{F}_R(\lambda_I) + 2(1-f)\mathcal{F}_I(\lambda_I)\,.$$

HB for Synchronous Mode III

Plot of τ_H (left) and λ_{IH} (right) versus D_0 for $f = 0.5$.





Key: No HB for synchronous mode when $D < D_{0c}$. Blowup as $D_0 \to D_{0c}^+$.

Main Result: Q.E. spot patterns linearly stable when $D_0 < D_{0c}\,, \forall\, \tau = \mathcal{O}(1)$.

Limiting Asymptotics: As $D_0 \to D_{0c}^+$, we have

$$\lambda_{IH} \sim \sqrt{\frac{D_0}{D_{0c}} - 1}\left(\frac{1}{(1-f)^2} - 2\kappa_c\right)^{-1/2}, \qquad \tau_H \sim \frac{\mu_0(1-f)}{\left(\frac{D_0}{D_{0c}} - 1\right)}\left(\frac{1}{(1-f)^2} - 2\kappa_c\right),$$

where $\mathcal{F}(i\lambda_I) \sim 1 + i\lambda_I - \kappa_c \lambda_I^2 + \cdots$ as $\lambda_I \to 0$ with $\kappa_c \approx 0.436$.

New (Modified) NLEP Problem

Warning: Conventional NLEP (based on $\tau\nu|\lambda|/D_0 \ll 1$) is invalid 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 $|\tau\lambda\nu/D_0| \gg 1$. Then, G_λ is closely approximated by the free-space Green's function G_f:

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

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

$$\tau \equiv \epsilon^{-\tau_c}/\nu\,, \qquad 0 < \tau_c < 2\,.$$

We readily calculate, with γ_e Euler's constant, that for each j:

$$2\pi\nu\kappa_j = -\frac{\tau_c}{2} + \nu\mathcal{K}_0\,, \qquad \mathcal{K}_0 \equiv -\frac{1}{2}\log\lambda + \log\left(2\sqrt{D_0}\right) - \gamma_e\,.$$

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

$$g(\lambda) \equiv \frac{1}{2} + \frac{(\lambda+1)}{2(1-f)\,(\lambda+1-f)}\,\frac{D_0\theta}{\left(1-\frac{\tau_c}{2}+\nu\mathcal{K}_0\right)} - \mathcal{F}(\lambda)\,.$$

Anomalous Scaling of a HB

To determine a HB we set $g(i\lambda_I) = 0$ and calculate τ_c.

Key: $\exists$ a root with $\lambda_I \ll 1$ (low frequency HB).

Main Result: [CTWW] *Let $D_0 < D_{0c}$, $\epsilon \ll 1$ with $\nu = -1/\log \epsilon$. 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:*

$$\tau_H \sim \frac{1}{\nu}\epsilon^{-\tau_c} \,,$$

$$\tau_c = 2\left(1 - \frac{D_0}{D_{0c}}\right) - \nu \log \nu + \nu \left(2 \log \left(2\sqrt{D_0}\right) - 2\gamma_e - \log \lambda_{I0}\right) + \mathcal{O}(\nu^2) \,,$$

$$\lambda = i\nu\lambda_{I0} + \mathcal{O}(\nu^3) \,, \qquad \lambda_{I0} \equiv \frac{\pi D_{0c}}{4D_0}(1-f) \,.$$

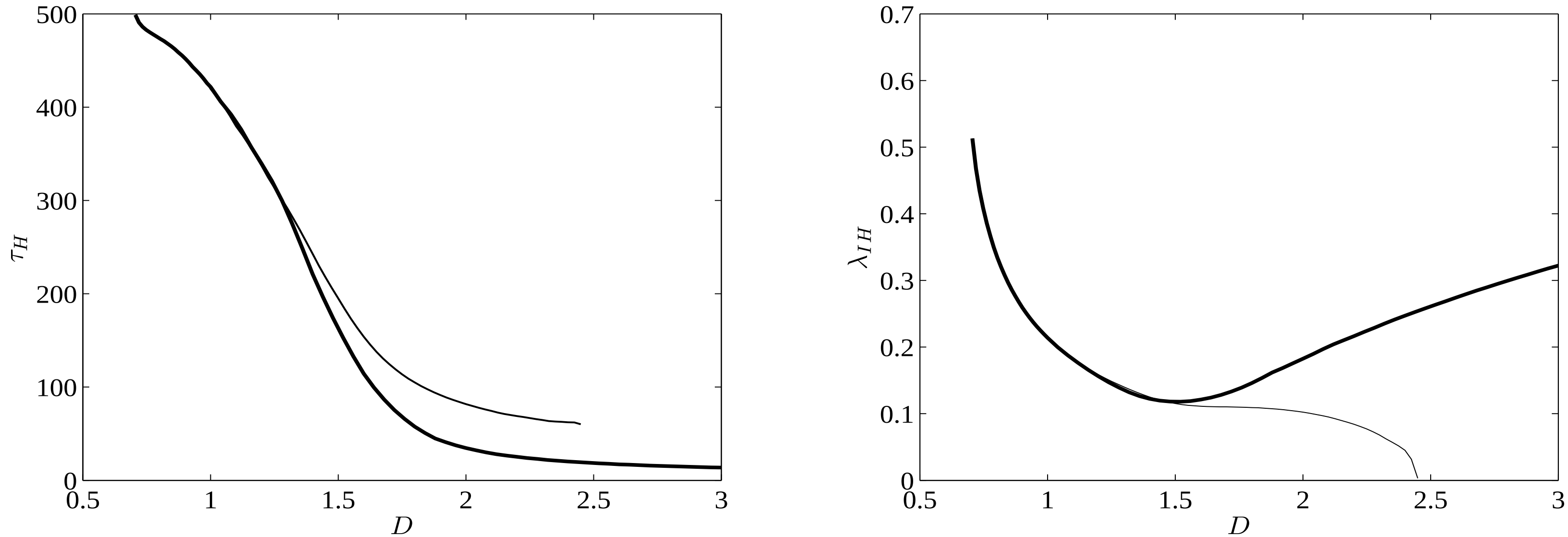
Remarks:

- The anomalous HB threshold is (asymptotically) the same $\forall j$.
- τ_c is independent of spot configuration. Spatial mode spans $\mathbb{R}^N$.
- Not uniformly valid as $D_0 \to D_{0c}^-$. In this limit we need NLEP with "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.

HB Threshold: Full Green's Matrix I

For D near D_{0c}/ν, the multipliers β_j of the NLEP involve the $\mathcal{G}_\lambda$ matrix and its matrix spectrum $\mathbf{c}_j$ (spatial modes) and eigenvalues κ_j.

Two-Spot Ring Pattern in Unit Disk: τ_H and λ_{IH}.



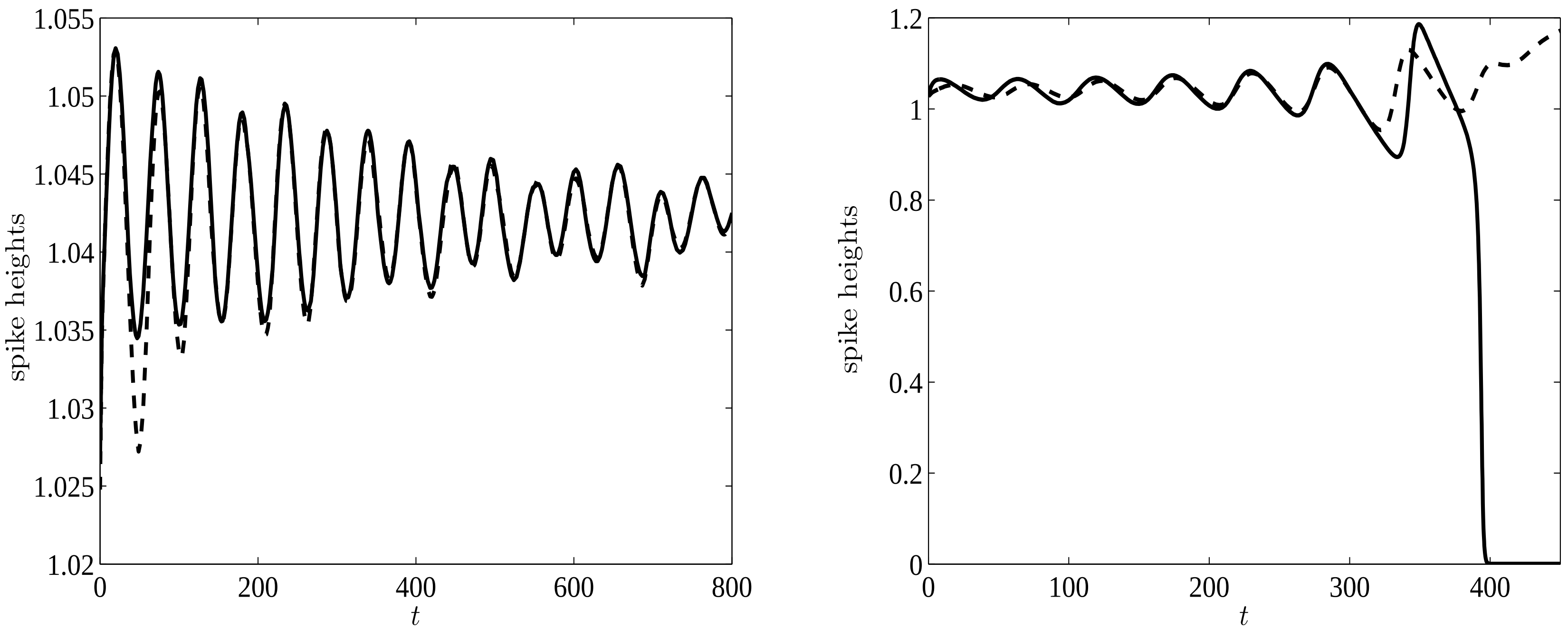
Caption: HB thresholds for $r_0 = 0.5$, $\epsilon = 0.02$, $f = 0.7$, and $E = 4$. The competition threshold is $D_c \approx 2.5$. Synchronous (heavy) and asynchronous (light).

Conventional NLEP: describes HB for $D > D_{0c}/\nu \gg 1$.
Modified NLEP: with anomalous scaling describes coalesence of HB for $D < D_{0c}/\nu$.
Full NLEP: with matrix $\mathcal{G}_\lambda$ when $D_0 \approx D_{0c}$ giving two distinct thresholds.

HB Threshold: Full Green's Matrix II

Validate: theory with full PDE numerical simulations from FlexPDE for two-spot ring pattern. $\mathcal{G}_\lambda$ is cyclic symmetric: $\mathbf{c}_1 = (1,1)^T$, $\mathbf{c}_2 = (1,-1)^T$.

Full Numerics for $D = 1.5$**:** $\tau = 150$ **(left)** $\tau = 170$ **(right).** $\tau_H \approx 163$ **(Sycn).**



Conjecture: Suggests subcritical HB. To date; no weakly nonlinear theory.

Refined Competition Threshold I

From a two-term-in-ν asymptotic expansion.....

Main Result ([CTWW]): (Finite Domain): *Let $\nu \ll 1$, $N \geq 2$, and suppose that the symmetry condition $\mathcal{G}_0 \mathbf{e} = \kappa_{01} \mathbf{e}$ on the spot configuration $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ holds. Then, for*

$$D = D_{0c}/\nu + D_1 + o(1)\,,$$

the spectrum of the NLEP for the competition modes has discrete eigenvalues λ near the origin, with $|\lambda| = \mathcal{O}(\nu) \ll 1$, given by

$$\lambda = 2\nu(1-f)\left[-\pi\kappa_{0j} + \frac{D_1}{2D_{0c}} + A\right] + \mathcal{O}(\nu^2)\,,$$

for some constant $A = A(f)$ defined in terms of w. Here κ_{0j} for $j = 2, \ldots, N$ are the eigenvalues of the Neumann Green's matrix $\mathcal{G}_0$ in the $N-1$ dimensional subspace

$$\mathcal{G}_0 \mathbf{q}_j = \kappa_{0j} \mathbf{q}_j\,, \quad j = 2, \ldots, N\,, \qquad \mathbf{q}_j^T \mathbf{e} = 0\,.$$

Upshot: $\lambda = 0$ at (possibly) $N-1$ distinct values of D:

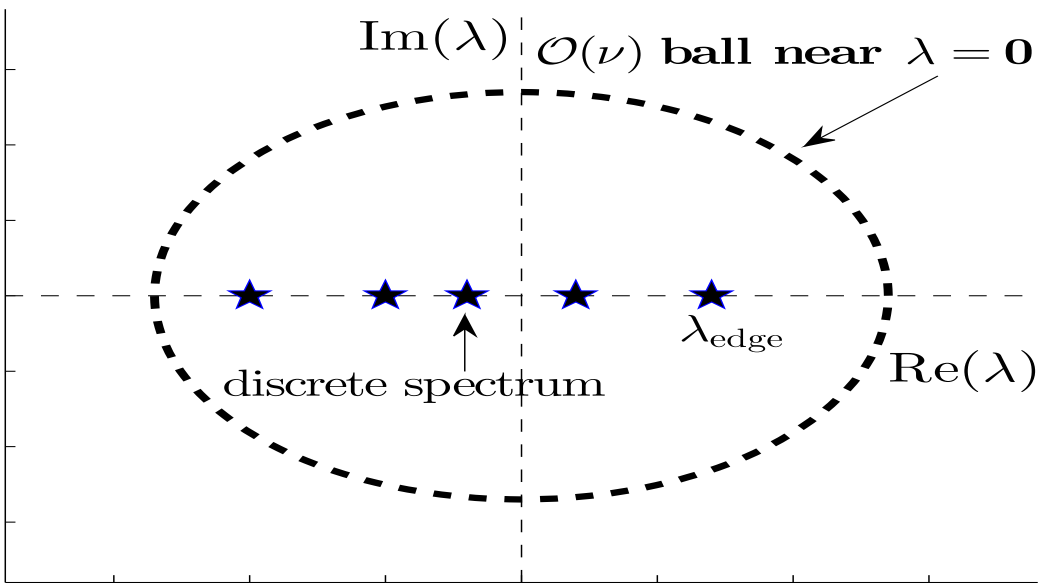
$$D \sim D_{j\epsilon} \equiv \frac{D_{0c}}{\nu}\left[1 + \nu\left(2\pi\kappa_{0j} - 2A\right)\right]\,, \quad j = 2, \ldots, N\,.$$

Refined Competition Threshold II

The competition instability threshold is

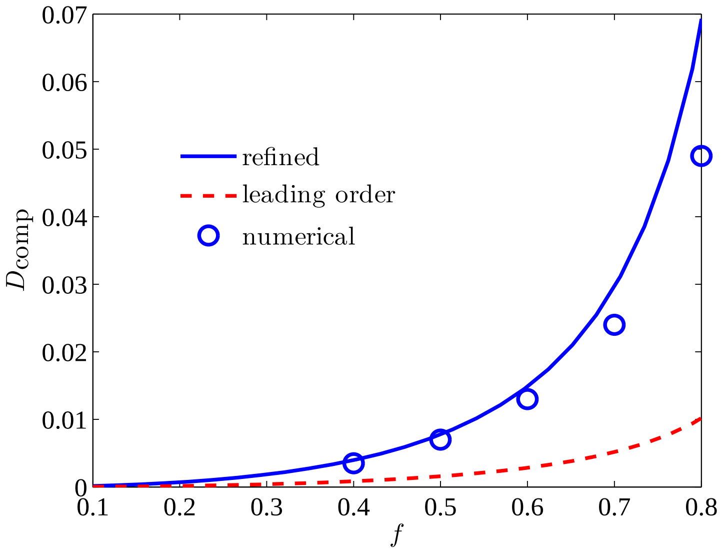
$$D_c \sim \frac{D_{0c}}{\nu}\left[1 + \nu\left(2\pi \kappa_{\text{min}} - 2A\right)\right] \,, \qquad \kappa_{\text{min}} \equiv \min_{j \in \{2,\ldots,N\}} \kappa_{0j} \,.$$

For the competition modes we have Re$(\lambda) < 0$ when $D < D_c$.

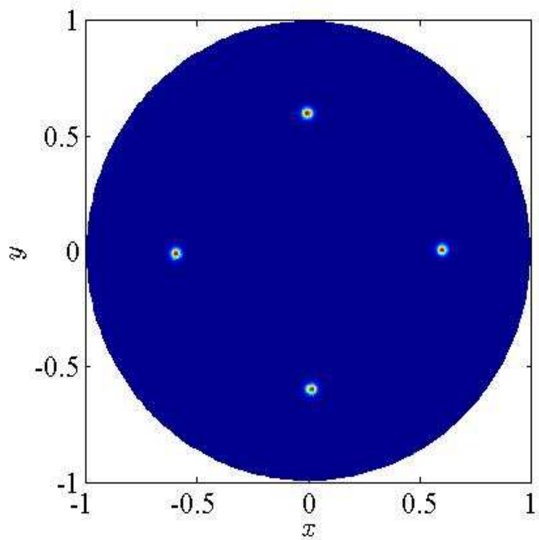


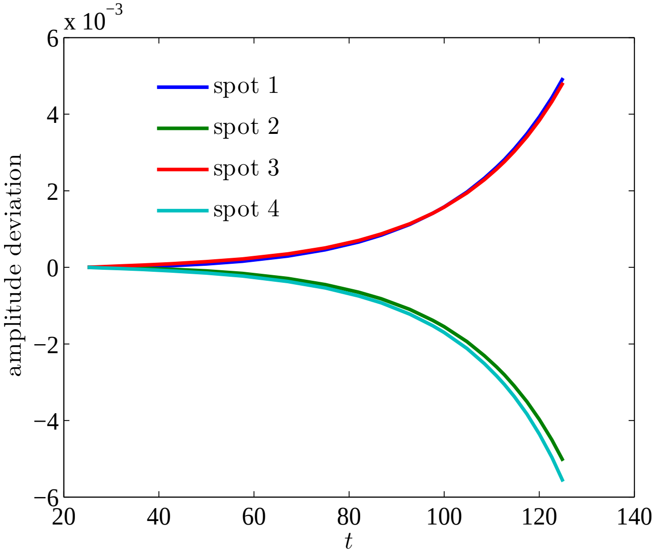
Caption: Discrete real eigenvalues with $|\lambda| = \mathcal{O}(\nu)$ when $\mathcal{G}_0$ has five distinct eigenvalues κ_{0j} in the subspace orthogonal to $\mathbf{e}$.

Refined Competition Threshold III



Numerical Validation: Four-spot ring pattern in unit disk.
Plot D_c versus f for ring radius $r_0 = 0.5986$, $\epsilon = 0.01$, and $E = 1$.



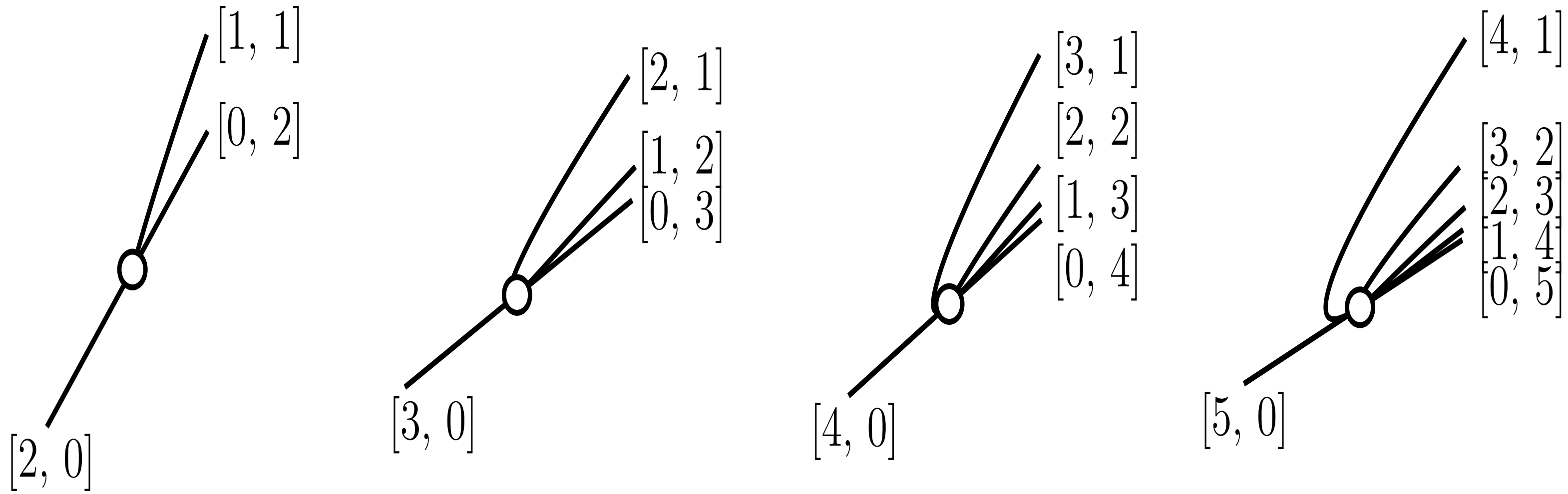


Left: surface plot of $v(\mathbf{x}, 0)$ **Right:** spot amplitudes (counterclockwise): dominant mode is $\mathbf{c} = (1, -1, 1, -1)^T$. Parameters: $f = 0.6$, $D = 0.014$, $\epsilon = 0.01$, $E = 1$, and $\tau = 0.002$.

Role of Symmetry Condition $\mathcal{G}_0\mathbf{e} = \kappa_{01}\mathbf{e}$: 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:

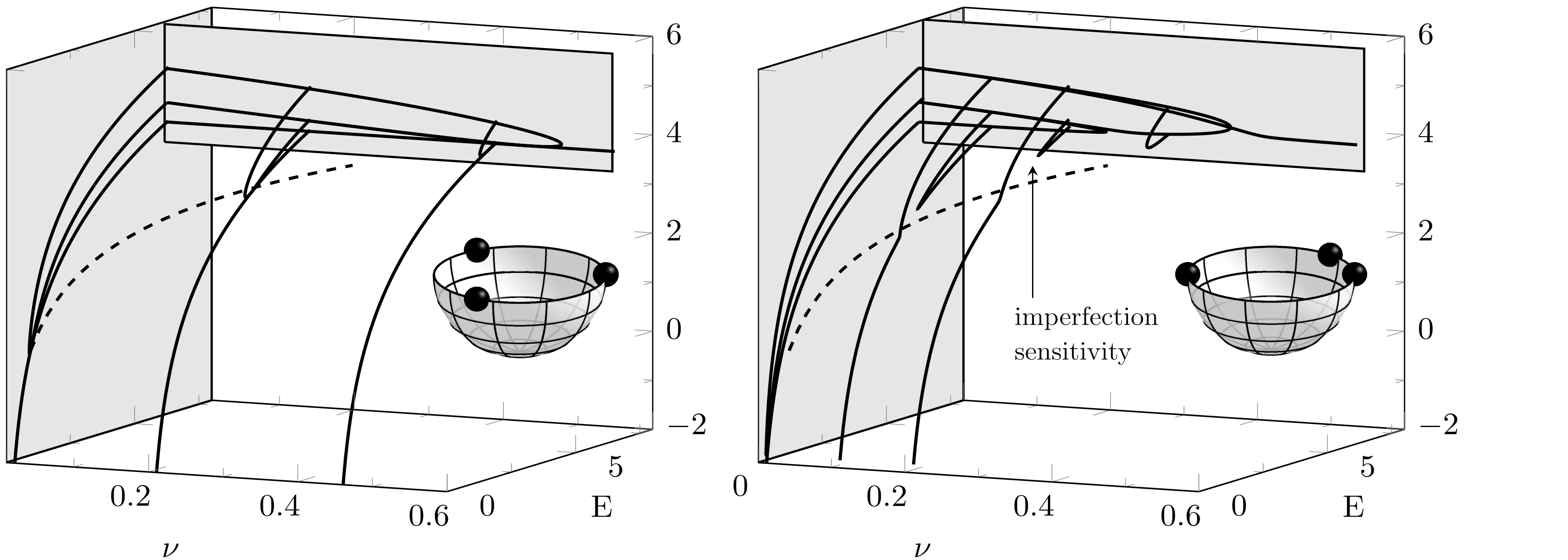


(a) $N = 2$ (b) $N = 3$ (c) $N = 4$ (d) $N = 5$

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

Role of Symmetry Condition $\mathcal{G}_0\mathbf{e} = \kappa_{01}\mathbf{e}$: II

Imperfection Sensitive if $\mathcal{G}_0\mathbf{e} \neq \kappa_{01}\mathbf{e}$. **Bif. Diag: 3-Spots on an Equator**



Accounting for all ν terms (summing the logs), spot quasi-equilibria determined from a nonlinear algebraic system (NAS) for the "spot source strengths $\mathbf{S} = (S_1, \ldots, S_N)^T$:

$$\mathbf{S} + 2\pi\nu\,(I - \mathcal{E})\,\mathcal{G}_0\mathbf{S} + \nu\,(I - \mathcal{E})\,\boldsymbol{\chi} = \frac{|\Omega|E}{2\pi N\sqrt{D}}\mathbf{e}\,.$$

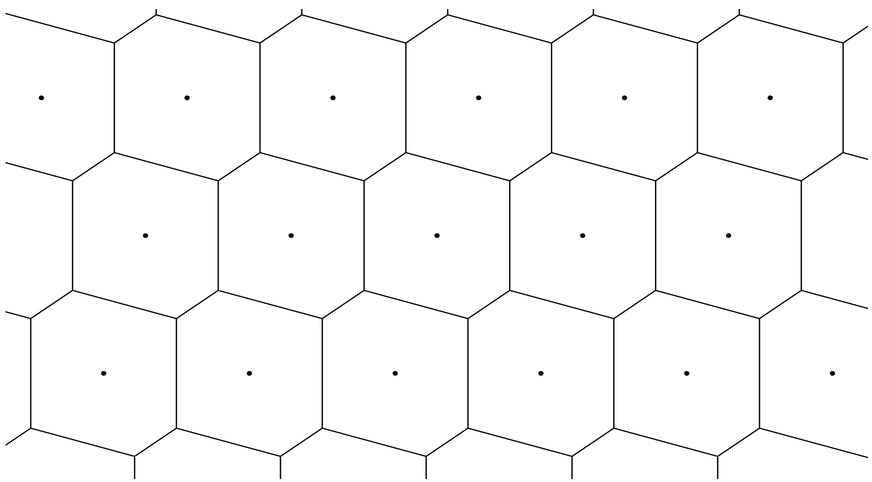
Key: If $\mathcal{G}_0\mathbf{e} = \kappa_{01}\mathbf{e}$, $\exists$ a solution with $\mathbf{S} = S_c\mathbf{e}$, with $S_c = |\Omega|E/(2\pi N\sqrt{D})$. Bifurcating branches at a critical value S_c* of S_c (competition threshold).

Periodic Spot Problem: Lattices I

Consider a periodic pattern of spots in $\mathbb{R}^2$ where the spots concentrate at lattice points of a Bravais lattice Λ:

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

WLOG, align $\boldsymbol{l}_1$ with positive x-axis. Fix $|\Omega| = 1$ as the area of the fundamental Wigner-Seitz cell centered at $\mathbf{x} = 0$. The WS cells tile $\mathbb{R}^2$.



Caption: WS cells for a lattice with $\boldsymbol{l}_1 = (1,0)$, $\boldsymbol{l}_2 = (\cot\theta, 1)$, $\theta = 74^\circ$, $|\Omega| = 1$.

Key Question: Consider $\mathcal{O}(1)$ time-scale instabilities due to spot amplitude instabilities. Which lattice offers the maximum competition threshold?

Lattices II

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:

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

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

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

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 calculating a required Bloch Green's function.

Periodic Spot Problem: II

Key Point: The leading-order threshold D_{0c} depends only on area $|\Omega|$ of FWS and is independent of the specific lattice. Need to "unfold" as

$$D = \frac{D_{0c}}{\nu} + D_1 + o(1)\,, \qquad D_{0c} \equiv \frac{|\Omega|^2 f^2 E^2}{4\pi^2 b(1-f)}$$

Strategy:

- Calculate the band of continuous spectrum satisfying $|\lambda| = \mathcal{O}(\nu) \ll 1$.
- For a given lattice Λ, choose D_1 sufficiently small so that the entire band satisfies Re$(\lambda) < 0$.
- Fix $|\Omega| = 1$. Maximize D_1 wrt Λ, to identify the "optimal" Λ.

Outline of Analysis:

- For $\epsilon \to 0$ construct a steady-state spot centered at $0 \in \Omega$. Extend.
- Linearize. For $\epsilon \to 0$, the eigenfunction Ψ for the long-range component u satisfies an elliptic PDE with coefficients that are periodic on Λ. Thus, by Floquet-Bloch, we impose $\Psi(\mathbf{x}+\boldsymbol{l}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{l}}\,\Psi(\mathbf{x})$.
- Formulate boundary operator $\mathcal{P}_k\Psi$ on $\partial\Omega$, so that Ψ related to Bloch Green's function G_{b0}:

Periodic Spot Problem: III

- The Bloch Green's function on WFS Ω for $\mathbf{k}/(2\pi) \in \Omega_B$ satisfies

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

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

  Here Ω_B is the first Brillouin zone of the dual lattice Λ^*

- Set $\lambda = \nu\lambda_1$. Calculate $\mathcal{O}(\nu)$ correction terms to leading-order NLEP. Impose solvability condition with adjoint to get λ_1.

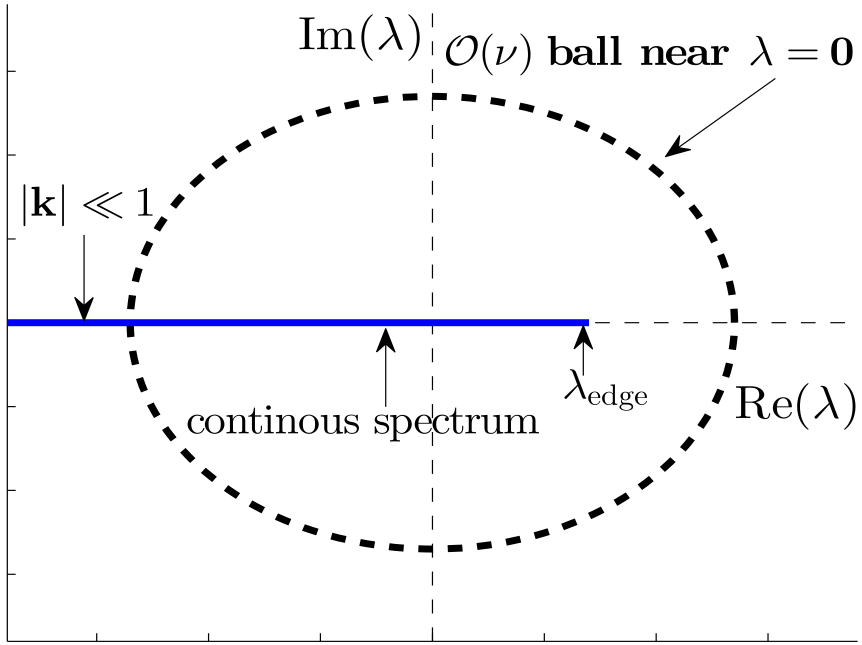
Main Result: [CTWW] *In the limit $\epsilon \to 0$, consider a steady-state periodic pattern of spots for the Brusselator where the spots are centered at the lattice points of a Bravais lattice Λ. Then, for $D = D_{0c}/\nu + D_1$, the portion of the continuous spectrum of the linearization satisfying $|\lambda| \leq \mathcal{O}(\nu) \ll 1$, is*

$$\lambda = 2(1-f)\nu \left[-\pi R_{b0}(\mathbf{k}) + \frac{D_1}{2D_{0c}} + A \right] + \mathcal{O}(\nu^2) \,.$$

Here $R_{b0}(\mathbf{k})$ is the regular part of G_{b0} and $A = A(f)$.

Periodic Spot Problem: IV

Plot of the Spectrum Near Criticality



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

Implication: For spot amplitude perturbations (governed by NLEP), long-wavelength $\mathbf{k} \to 0$ perturbations are “safe”.

Periodic Spot Problem: V

Key Conclusion: a periodic pattern of spots on a fixed lattice Λ is linearly stable on $\mathcal{O}(1)$ time-scales when

$$D_1 < D_1^\star \equiv D_{0c}\left[2\pi R_{b0}^\star - 2A\right], \quad R_{b0}^\star \equiv \min_{\mathbf{k}/(2\pi)\in\Omega_B} R_{b0}(\mathbf{k}).$$

The optimal lattice Λ_{opt} is the one for that solves the variational problem:

$$\max_{\Lambda} R_{b0}^\star$$

From an Ewald-type analysis relying on the Poisson summation formula (cf. Beylkin (2008)) we calculate (with $\eta > 0$ the Ewald parameter)

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

where $F_{\text{sing}}(\boldsymbol{l}) = E_1(|\boldsymbol{l}|^2\eta^2)/(4\pi)$ and E_1 is the exponential integral. Here $\eta > 0$ is used for rapid convergence of the two infinite sums.

Numerics of R_{b0} of Bloch G-Function

Goal: Determine the lattice arrangement that maximizes $R_{b0}^\star$, where $R_{b0}^\star = \min_{\mathbf{k}/(2\pi)\in\Omega_B} R_{b0}(\mathbf{k})$.

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 $|\Omega| = 1$.

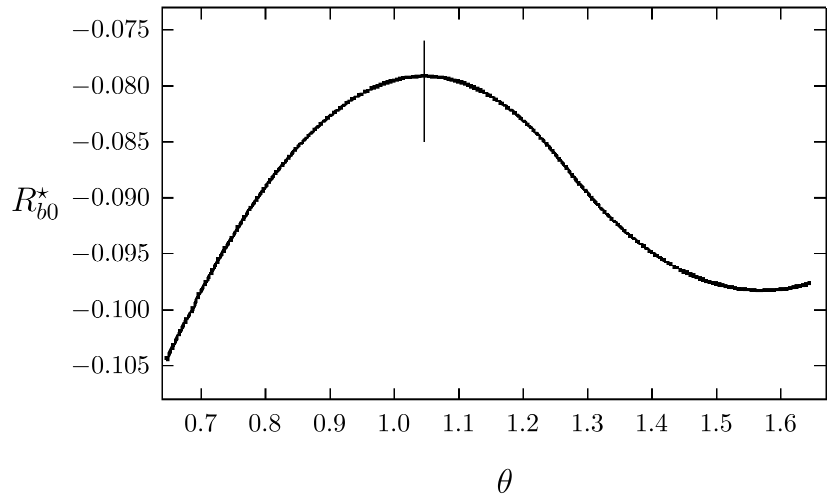
Sweeping over Ω: Numerical Computations of R_{b0}

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 $\theta = \pi/3$.

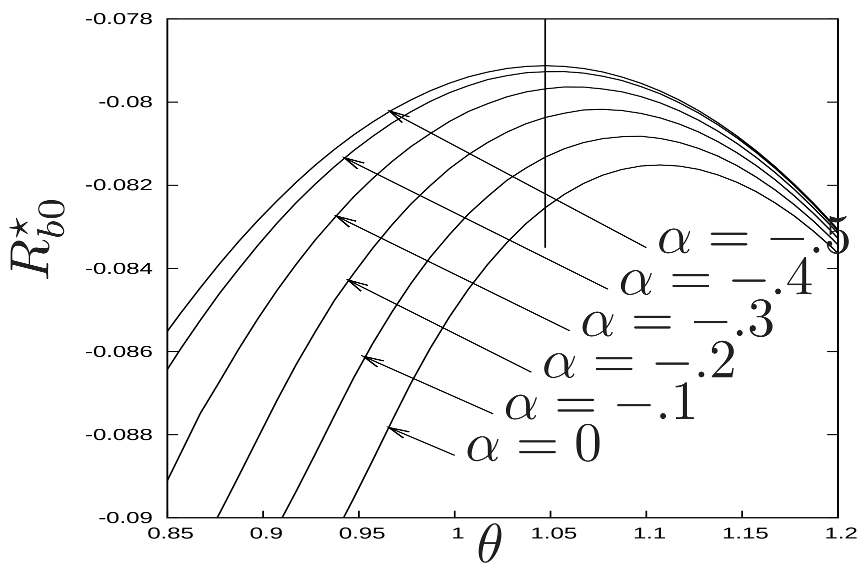
Sweep II: Let $\boldsymbol{l}_1 = (a, 0)$ and $\boldsymbol{l}_2 = (b, c)$, and introduce parameter α. Define $a = (\sin\theta)^\alpha$, $c = (\sin\theta)^{-\alpha}$ and $b = \cos\theta\ (\sin\theta)^{-\alpha-1}$. Then, $|\Omega| = 1$. Note: regular hexagon occurs only when $\alpha = -0.5$ (at $\theta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

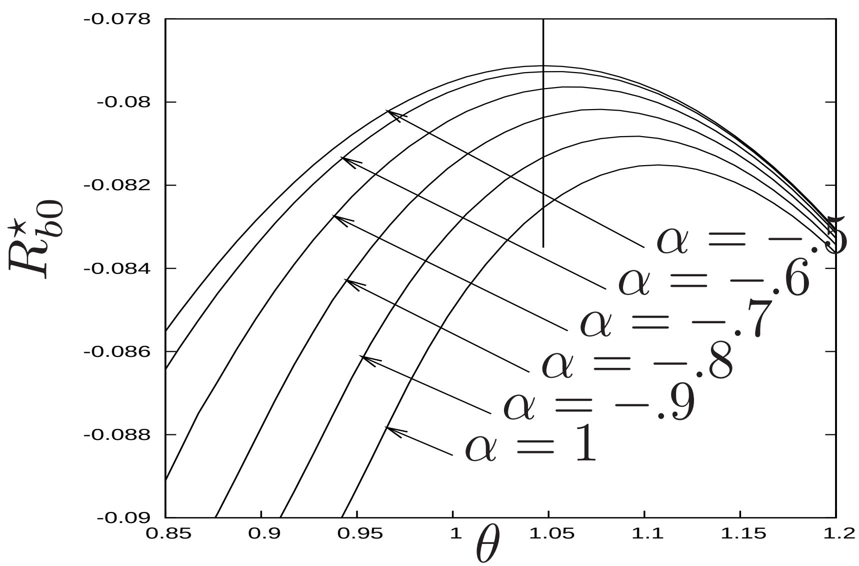
Numerical Computation of Optimal R^*_{b0}

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



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





GM: Main Result for Periodic Patterns

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

Main Result: [IRWW] *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*

$$\lambda = \nu \lambda_1 + \cdots \,, \quad \lambda_1 = \mu_1 - 4\pi R_{b0}(\mathbf{k}) + 2\pi R_{0p} - B \,,$$

where R_{0p} is the regular part of the periodic source-neutral G-function on WS cell. Periodic pattern on Λ is linearly stable when

$$\mu_1 < \mu_1^{\star} \equiv 4\pi R_{b0}^{\star} - 2\pi R_{0p} + B \,, \quad R_{b0}^{\star} \equiv \min_{\mathbf{k}/(2\pi) \in \Omega_B} R_{b0}(\mathbf{k}) \,.$$

The optimal lattice arrangement maximizes $\mathcal{K}_{gm} \equiv 4\pi R_{b0}^{\star} - 2\pi R_{0p}$. The stability threshold on the optimum lattice is

$$D_{\text{optim}} \sim \frac{|\Omega|}{2\pi\nu} \left[1 + \nu \left(\max_{\Lambda} \mathcal{K}_{\text{gm}} + B \right) \right] \,.$$

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

Main Result: [IRWW] Regular hexagon is the optimal lattice.

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.
- 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 $\mathcal{O}(\epsilon^2)$ (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: Final Remark

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

References: Available at http://www.math.ubc.ca/∼ward

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