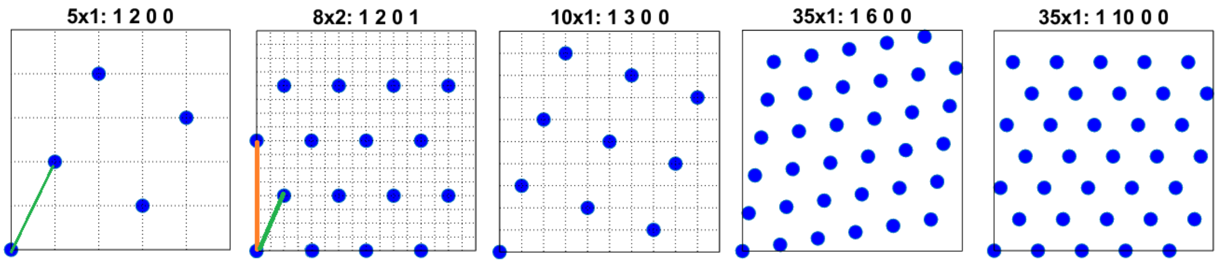
Pattern formation on a periodic rectangle



(a) (b) (c) (d) (e)

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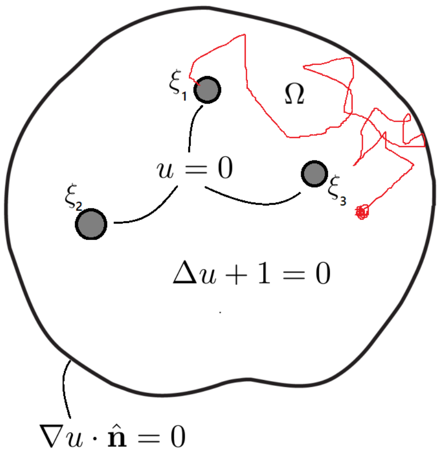
Two related problem:

- **Problem A:** Mean First Passage Time (MFPT) inside a reflective domain with small traps:

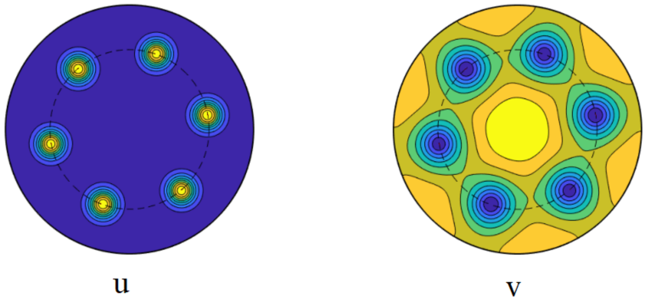


  - ***What are optimal trap locations to minimize MFPT?***

- **Problem B:** Spike patterns in Schankenberg (and similar) RD model:

$$u_t = \varepsilon^2 \Delta u - u + u^2 v, \qquad 0 = \Delta v + A - u^2 v \frac{1}{\varepsilon^2} \frac{1}{\log \varepsilon^{-1}} \tag{1}$$

– Example of a stable equilibrium:



– ***Where are stable spike locations?***

Green potential

- Define the Modified Green's function to solve

$$\Delta G - \frac{1}{|\Omega|} + \delta\,(x-y) = 0; \quad \int_\Omega G = 0, \quad \partial_n G = 0 \text{ on } \partial\Omega; \tag{2}$$

and the Regular part of G:

$$R(x,y) = G(x,y) + \frac{1}{2\pi}\log|x-y|\,. \tag{3}$$

- Define **Green's function interaction potential (or energy)** to be

$$E\,(\xi_1,\ldots\xi_N) := \sum_{k=1}^{N}\left(R(\xi_k,\xi_k) + \sum_{j\neq k}^{N} G(\xi_k,\xi_j)\right). \tag{E}$$

- Corresponding gradient flow (steepest descent) is:

$$\frac{d}{dt}\xi_k = -\nabla_1 R(\xi_k,\xi_k) - \sum_{j\neq k}\nabla_1 G(\xi_k,\xi_j) \tag{flow}$$

- ***Optimal trap locations for MFPT problem correspond to minima of E***

- ***Spike motion for the Schnakenberg model follows (flow) (in certain limits)***
  - Stable spike equilibria locations correspond to stable equilibria of (flow), or local minima of E.

- **Question: classify situations for which minimizers of E have analytic solution.**

Periodic rectangle

- Consider a Green's function on a rectangle with periodic BC:

$$\Omega = \{(x, y) : 0 \le x \le L, 0 \le y \le H\},$$

$$\Delta G - \frac{1}{|\Omega|} + \delta(x) = 0; \quad \int_\Omega G = 0; \quad G \text{ is } \textbf{periodic} \text{ on } \partial\Omega. \tag{4}$$

- Define the energy to be

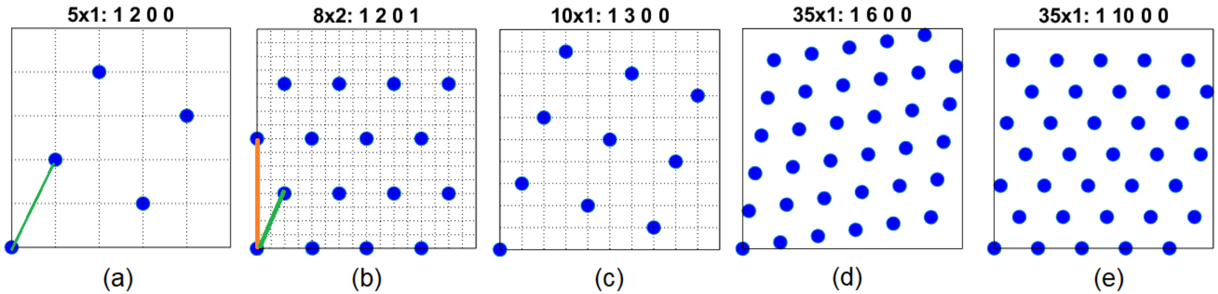
$$E(\xi_1, \ldots \xi_N) := \sum_{k=1}^{N} \sum_{j=k+1}^{N} G(\xi_k - \xi_j); \tag{5}$$

and gradient flow:

$$\frac{d}{dt}\xi_k = -\sum_{j \ne k} \nabla G(\xi_k - \xi_j) \tag{6}$$

- An integer lattice of size N has the form:

$$N = n_1 n_2; \quad \tilde{L} = \{(a,b)\, n_2 j_1 + (c,d) n_1 j_2 \pmod{N} : j_1 \in \mathbb{Z}_{n_1}, \quad j_2 \in \mathbb{Z}_{n_2}\} \tag{7}$$



From an integer lattice of N points, we obtain a ***regular lattice*** inside the rectangle Ω :

$$L = \left\{ \left(x\frac{L}{N}, y\frac{H}{N} \right) : (x,y) \in \tilde{L} \right\} \tag{8}$$

- **Theorem:** ***Every regular lattice is a critical point*** of E (but most are saddles, not local minima)
  - Due to the high symmetry of the lattice, and the fact that G is even.

- A ***stable*** lattice on a rectangle $(0,L)\times(0,H)$ is a lattice which is a local minimum of E, or equivalently, a stable equilibrium of flow (6)

Classifying integer lattices

- [Hanany, Orlando, Reffert, 2010]: Number of non-equivalent lattices on a square with N points has a generating function:

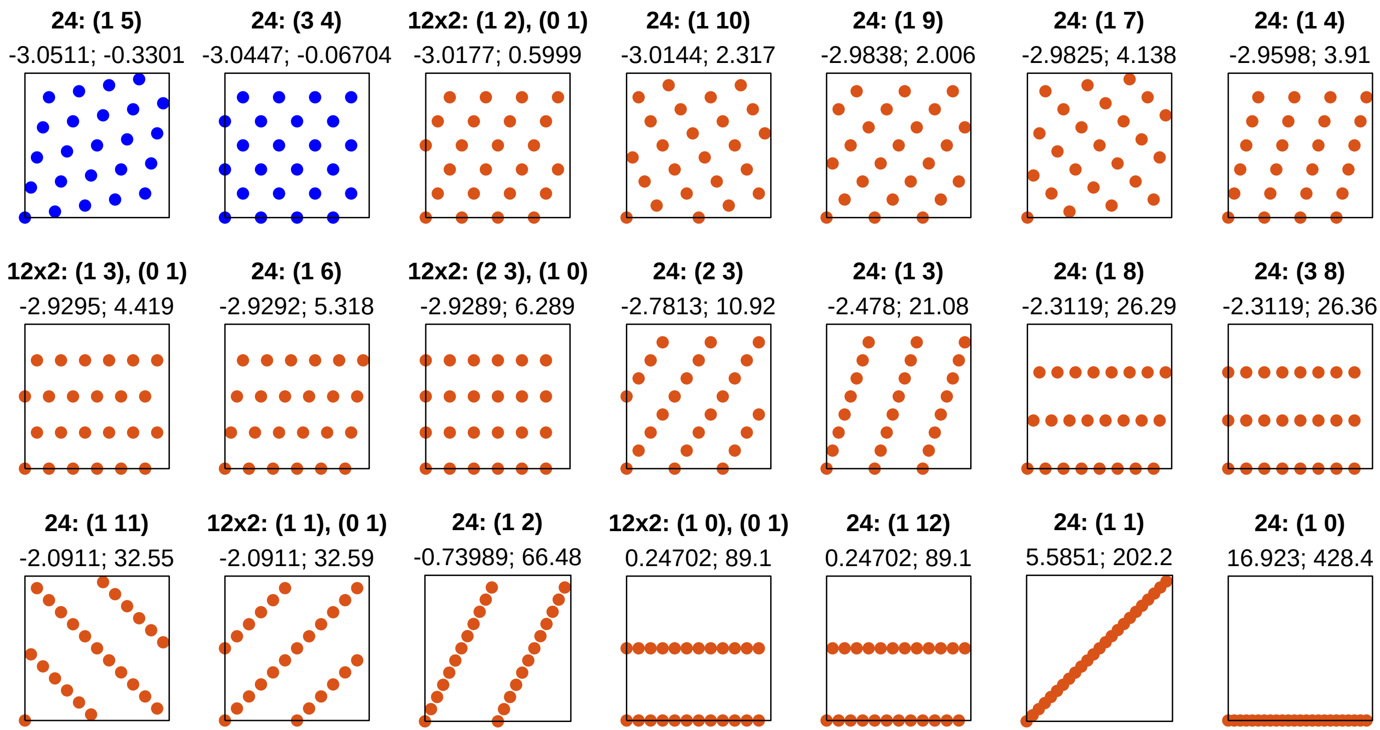
$$\sum_{m=1}^{\infty}\left[\frac{1}{(1-t^{m})(1-t^{4m})}-1\right]$$

N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	...	24	...	30
#lattices	1	2	3	5	4	7	5	10	8	10	4	11	5	8	8	12		21		22

- **Question:** How many of these are ***stable on a square*** $(H = L)$? How does the ***aspect ratio*** H/L affect stability?

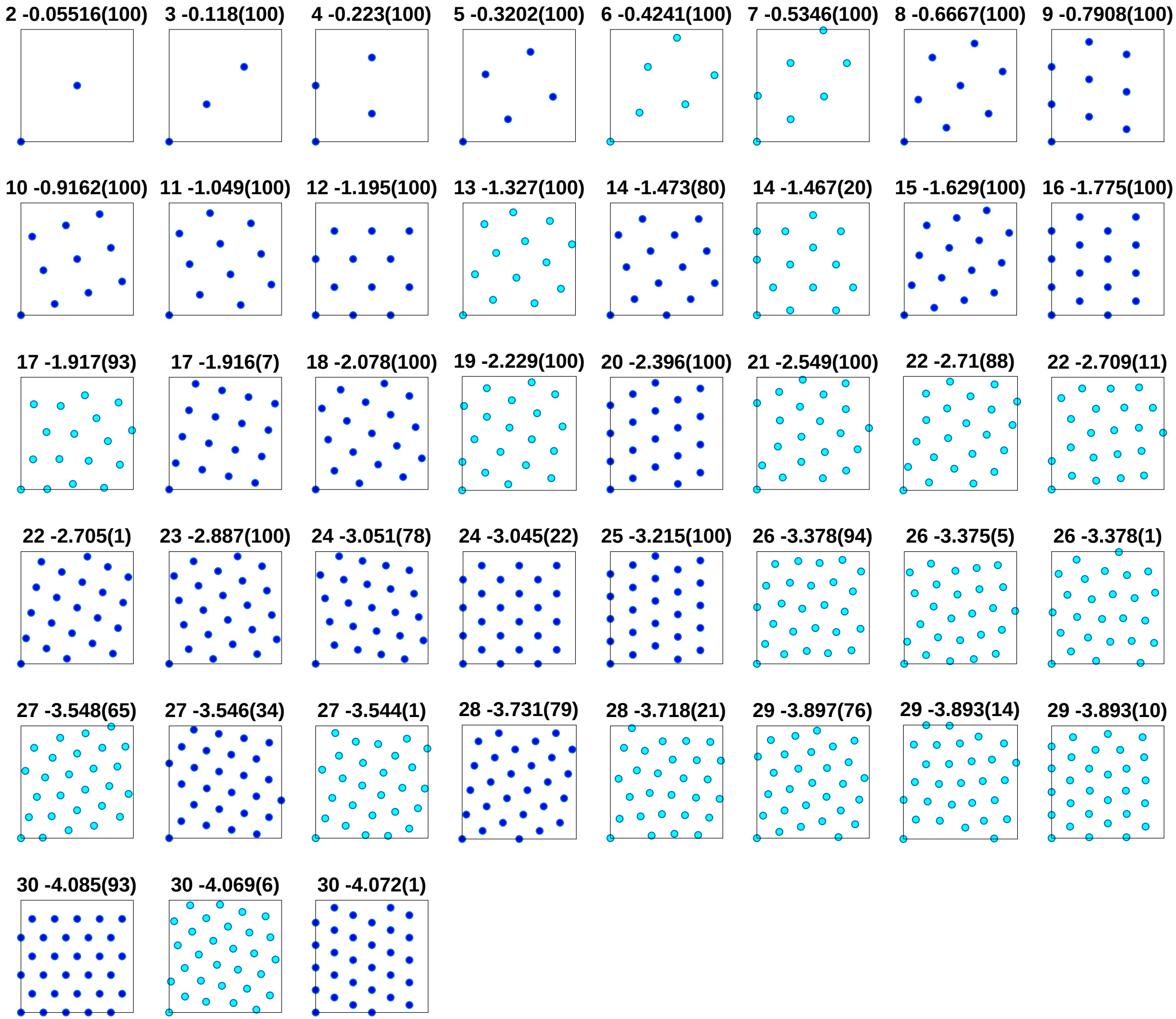
Example: $N = 24$

- 21 distinct lattices on a square, only two are stable.



- Example of (1,5) stable spot pattern for Schank: Movie

Regular lattice v.s. irregular equilibria



Formula for stability of a lattice

- Let v_1, v_2 be the basis vectors. Let v is the 2x2 matrix $(v_1|v_2)$. Lattice points are:

$$\xi_j = \xi_{(j_1,j_2)} = vj = v_1 j_1 + v_2 j_2 \pmod{\Omega}, \quad j \in \mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2}. \tag{9}$$

  The gradient flow becomes

$$x'_k = \sum_{j \neq k} G_1(x_j - x_k, y_j - y_k)$$
$$y'_k = \sum_{j \neq k} G_2(x_j - x_k, y_j - y_k).$$

  Here, the indices represent vectors $k = (k_1, k_2)^T$ and $j = (j_1, j_2)^T \in Z_{n_1 \times n_2}$, and $\sum$ is the double sum having $n_1 n_2 - 1$ terms; and we denoted $G_1(x, y), G_2(x, y)) = \nabla G(x, y)$.

- Linearize

$$x_k(t) = vk + e^{\lambda t}\phi_k, \quad y_k(t) = vk + e^{\lambda t}\psi_k,$$

  to obtain $2N \times 2N$ eigenvalue problem

$$\lambda \phi_k = \sum_{j \neq k} G_{11}(v\,(j-k))\,(\phi_j - \phi_k) + G_{12}(v\,(j-k))\,(\psi_j - \psi_k)$$
$$\lambda \psi_k = \sum_{j \neq k} G_{21}(v\,(j-k))\,(\phi_j - \phi_k) + G_{22}(v\,(j-k))\,(\psi_j - \psi_k)$$

- **Fourier-like decomposition**: Let $m = (m_1, m_2) \in \mathbb{Z}_{n_1 \times n_2}$ and define

$$\phi_k = \exp\left\{2\pi i \left(\frac{m_1}{n_1}k_1 + \frac{m_2}{n_2}k_2\right)\right\}\phi, \quad \psi_k = \exp\left\{2\pi i \left(\frac{m_1}{n_1}k_1 + \frac{m_2}{n_2}k_2\right)\right\}\psi \tag{10}$$

Here $(m_1, m_2) \in \mathbb{Z}_{n_1 \times n_2}$, are a pair of Floquet multipiers or modes. This yields a 2x2 eigenvalue problem

$$\lambda_{(m_1,m_2)} \begin{pmatrix} \phi \\ \psi \end{pmatrix} = M \begin{pmatrix} \phi \\ \psi \end{pmatrix}, \quad \text{where} \ \ M = \begin{bmatrix} M_{11} & M_{21} \\ M_{12} & M_{22} \end{bmatrix}, \tag{11}$$

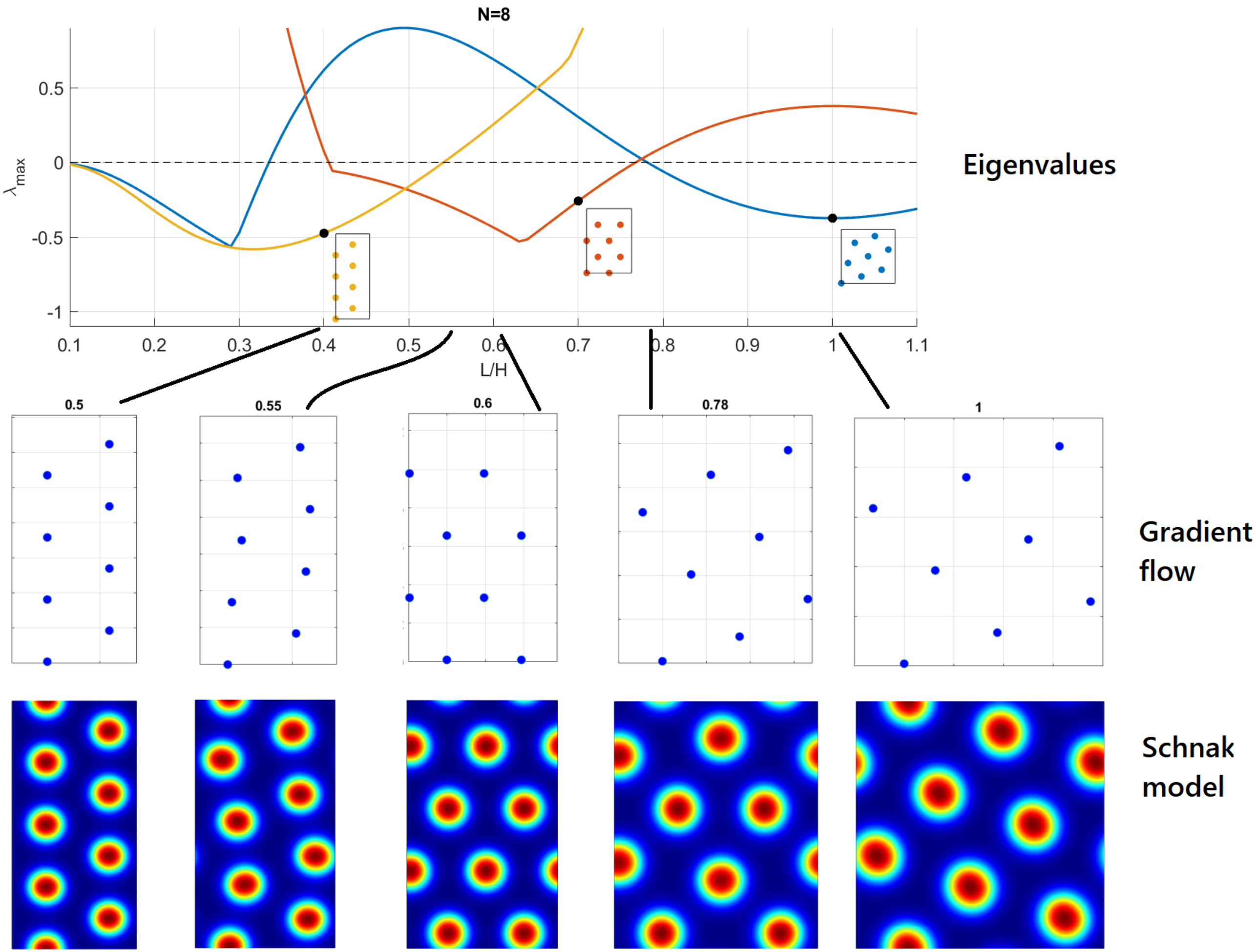
$$M_{a,b} = \sum_{l \in \mathbb{Z}_{n_1 \times n_2} \backslash (0,0)}^{n-1} G_{ab}(vl)\left(\exp\left\{2\pi i \left(\frac{m_1}{n_1}l_1 + \frac{m_2}{n_2}l_2\right)\right\} - 1\right). \tag{12}$$

- Algorithm to determine stability:
  - Generate all possible lattices
  - For each lattice:
    * compute N eigenvalues $\lambda_{(m_1,m_2)}$
    * If there exists $\lambda_{(m_1,m_2)} > 0$ then it is unstable, otherwise stable.

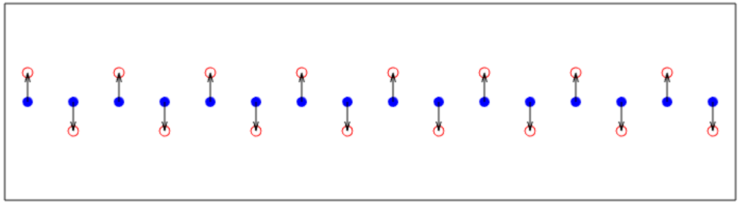
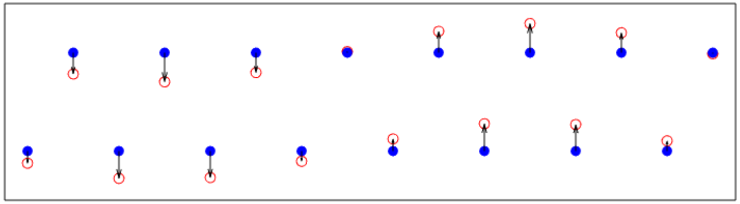
Results

N	#all	#stable	N	#all	#stable	N	#all	#stable	N	#all	#stable
1	1	1	26	13	0	51	20	0	76	39	3
2	2	1	27	12	1	52	29	2	77	26	3
3	2	1	28	18	2	53	15	2	78	46	1
4	4	1	29	9	0	54	34	1	79	21	1
5	3	1	30	22	2	55	20	0	80	55	3
6	5	0	31	9	0	56	36	2	81	33	3
7	3	0	32	21	1	57	22	1	82	34	2
8	7	1	33	14	1	58	25	1	83	22	1
9	5	1	34	16	1	59	16	2	84	64	3
10	7	1	35	14	2	60	50	3	85	30	1
11	4	1	36	29	2	61	17	1	86	35	3
12	11	1	37	11	0	62	26	1	87	32	1
13	5	0	38	17	2	63	29	3	88	51	2
14	8	1	39	16	2	64	38	4	89	24	0
15	8	1	40	29	2	65	24	0	90	65	5
16	12	1	41	12	0	66	40	2	91	30	2
17	6	1	42	28	2	67	18	1	92	46	1
18	13	1	43	12	1	68	36	3	93	34	2
19	6	1	44	25	0	69	26	2	94	38	3
20	15	1	45	23	3	70	40	3	95	32	2
21	10	0	46	20	1	71	19	0	96	73	3
22	11	1	47	13	1	72	58	4	97	26	1
23	7	1	48	39	2	73	20	1	98	46	2
24	21	2	49	16	1	74	31	1	99	42	2
25	10	1	50	27	2	75	34	2	100	61	4

Varying aspect ratio



Single and double stripe

- Single stripe:
  - Always unstable; the dominant mode is high-frequency mode as shown.
- Double stripe (even N):
  - Generated by $v_1 = \left(\frac{1}{H}, \frac{N}{2L}\right)$;
  - Can be either stable or unstable depending on aspect ratio
  - Dominant instability corresponds to the mode $m_1 = 1$ as shown (lowest-frequency)

- **Proposition.** Consider the double-stripe as shown with $N = 2n$ spots with $n \gg 1$. Let $a \approx \mathbf{4.1485}$ be the root of

$$\sum_{j=1}^{\infty} \frac{(-r)^j}{\left(1-(-r)^j\right)^2} j^2 = 0; \qquad \exp(2\pi/a) = r \tag{13}$$

  There is a bifurcation at $\frac{N}{L}H = a$. The pattern is ***stable*** if $\frac{N}{L}H \leq a$ and is ***unstable*** otherwise.

- The derivation uses an explicit representation of the Green's function

$$G(x,y) = -\frac{L}{24H} + \frac{1}{2HL}(x - L/2)^2 + \sum_{q=1}^{\infty} \cos\left(2\pi q \frac{y}{H}\right) \frac{\cosh\left((x - L/2)\frac{2\pi}{H}q\right)}{2\pi q \sinh\left(\frac{2\pi}{H} q L/2\right)}$$

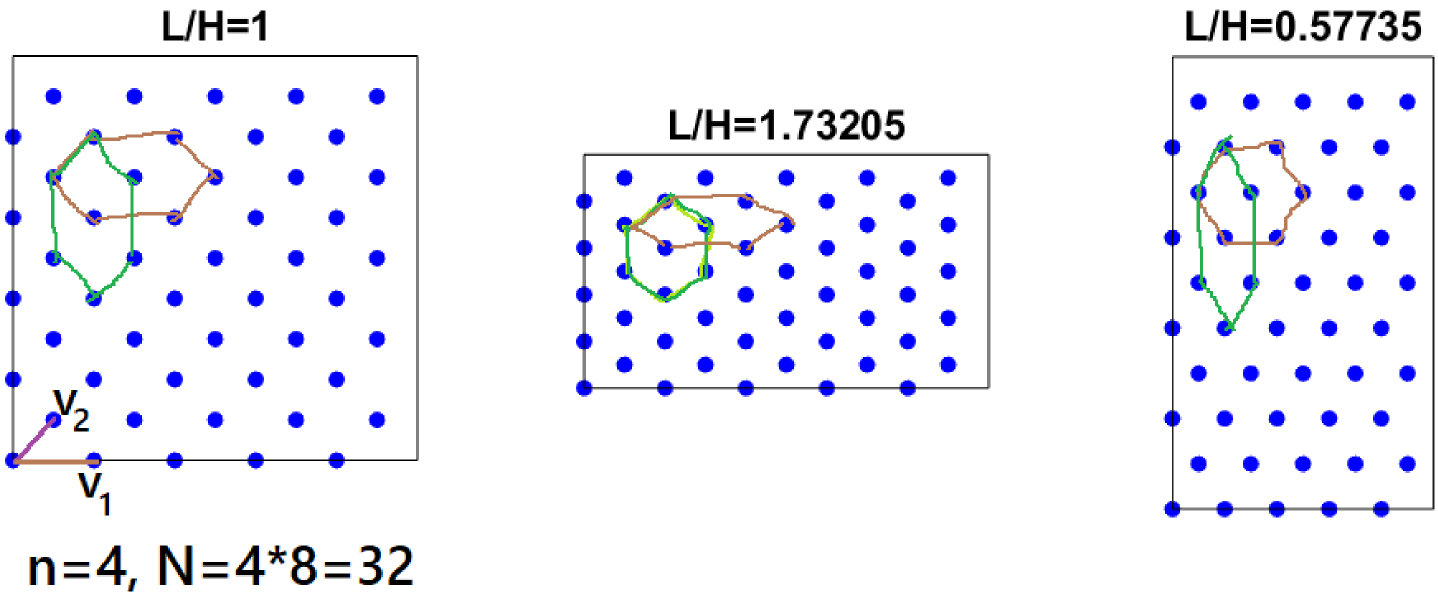
  as well as resummation tricks.

- Numerics: ***supercritical bifurcation*** to a "wavy state": 0.85*a →1.05*a
  - Followed by ***subcritical*** bifurcation back to regular lattice: →1.15*a

Hexagonal lattice

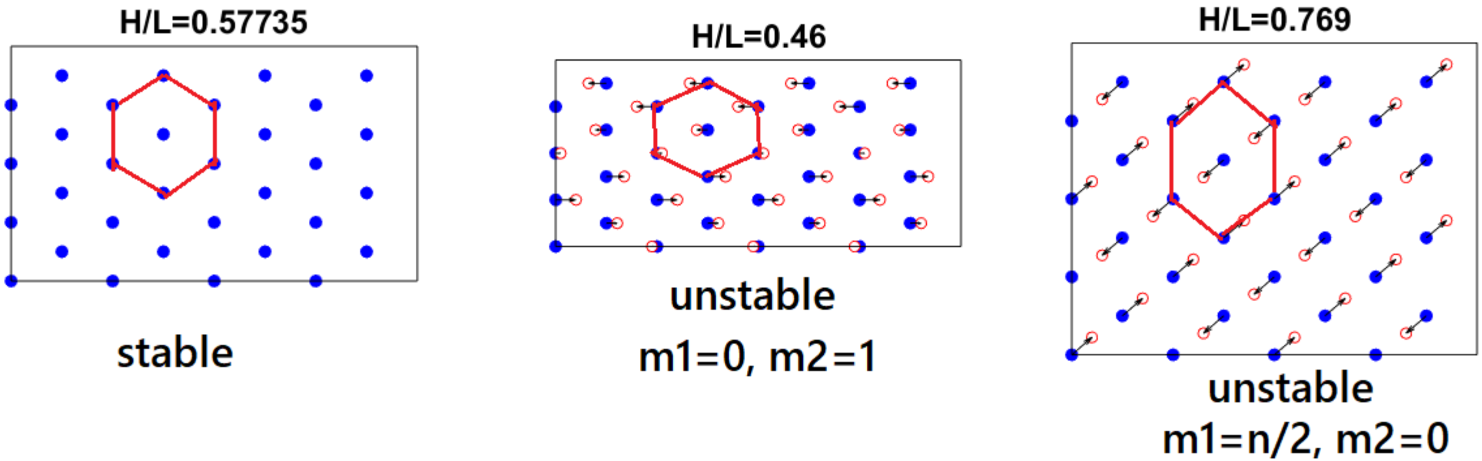
- Consider the regular lattice:

$$v_1 = \frac{1}{n}(L,0); \quad v_2 = \frac{1}{2n}(L,H); \quad v = (v_1|v_2);$$
$$x_{j_1 j_2} = vj, \quad j = (j_1, j_2) \in \mathbb{Z}_n \times \mathbb{Z}_{2n}, \quad N = 2n^2.$$



- It is a ***hexagonal lattice*** when $H/L = \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ (i.e. 30 or 60 degree angle between v_1 and v_2).

- **Main result:** In the limit $n \to \infty$, the lattice is stable when H/L or $L/H \in (0.4821, 0.7678)$ (angle between 25.73 and 37.52 degrees). At the boundaries, the dominant instability modes are:



  - When $H/L = 0.4821$,the mode is $(m_1, m_2) = (1, 0)$ becomes unstable. The value $\rho = 0.4821$ is the root of

$$0 = \sum_{j=1}^{\infty} \sum_{Q=1}^{\infty} Qj^2 \exp\left(-j\pi\rho Q\right) \cos\left(\pi Qj\right) \tag{14}$$

  - When $H/L = 0.7678$ the mode is $(m_1, m_2) = (1, 0)$ becomes unstable. The value $\rho = 0.7678$ is the root of

$$\left(f_1(\rho) - \frac{1}{8}\right)\left(-f_1(\rho) + \frac{1}{8} - \frac{1}{\pi\rho}\right) - f_2^2(\rho) = 0, \text{ where} \tag{15}$$

$$f_1(\rho) = \sum_{j=1}^{\infty} \sum_{Q=1}^{\infty} Q \exp\left(-j \frac{\pi}{2} \rho Q\right) \cos\left(\pi Q \left(1 + \frac{j}{2}\right)\right) \tag{16}$$

$$f_2(\rho) = \sum_{j=1}^{\infty} \sum_{Q=1}^{\infty} Q \exp\left(-j \frac{\pi}{2} \rho Q\right) \sin\left(\pi Q \left(1 + \frac{j}{2}\right)\right). \tag{17}$$

– Numerics: 0.7578 is supercritical, 0.4821 is subcritical:

– Movies, Schank: H/L=0.57 H/L=0.78, H/L=0.43

Under the hood

Mode $m_1 = 0, m_2 = 1$: Start with M_{11}

$$M_{11} = \sum_{l \in \mathbb{Z}_{n_1 \times n_2} \setminus (0,0)}^{n-1} G_{xx}(vl) \left(\exp\left\{ 2\pi i \left(\frac{m_1}{n_1} l_1 + \frac{m_2}{n_2} l_2 \right) \right\} - 1 \right)$$

$$G_{xx} = -\frac{2\pi}{L^2} \sum_{q=1}^{\infty} q \cos\left(2\pi q \frac{x}{L} \right) \frac{\cosh\left((y - H/2) \frac{2\pi}{L} q \right)}{\sinh\left(\frac{2\pi}{L} q H/2 \right)}. \tag{18}$$

$$x_j = \frac{L}{n} \left(j_1 + \frac{j_2}{2} \right), \; y_j = \frac{H}{n} \frac{j_2}{2}$$

$$M_{11}(m) = -\frac{2\pi}{L^2} \sum_{j_1=0}^{n_1-1} \sum_{j_2=1}^{n_2-1} \sum_{q=1}^{\infty} q \cos\left(2\pi q \frac{x_j}{L} \right) \frac{\cosh\left((y_j - H/2) \frac{2\pi}{L} q \right)}{\sinh\left(\frac{2\pi}{L} q H/2 \right)} \left(\exp\left\{ \frac{\pi i}{n} j_2 \right\} - 1 \right)$$

Sum over j_1 ***first***:

$$\sum_{j_1=0}^{n_1-1} \cos\left(\frac{2\pi q}{n} \left(j_1 + \frac{j_2}{2} \right) \right) = \left\{ \begin{array}{c} 0, \quad n|q \\ n \cos\left(\frac{\pi q}{n} j_2 \right), \quad n \not| q \end{array} \right.$$

Use asymptotics:

$$\frac{\cosh\left(\left(y_j - H/2\right)\frac{2\pi}{L}q\right)}{\sinh\left(\frac{2\pi}{L}qH/2\right)} \sim \exp\left(-y_j\frac{2\pi q}{L}\right), \quad q \text{ large}$$

We get:

$$M_{11}(m) \sim \frac{2\pi^2}{L^2}\sum_{j_2=1}^{\infty}\sum_{Q=1}^{\infty} Q\cos\left(\pi Q j_2\right)\exp\left(-j_2\pi\frac{H}{L}Q\right)j_2^2.$$

We also find $M_{22} < 0, \quad M_{12} = M_{21} = 0$, so that $\lambda = M_{11}$.

Theorem. Let

$$f(z) = \sum_{j=1}^{\infty}\sum_{Q=1}^{\infty} Q\cos\left(\pi Q j\right)\exp\left(-j\pi z Q\right)j^2 \tag{19}$$

, and let z_c be the root of $f(z)$. Then it's unstable when $H/L > z_c$.

Numerically, we have $z_c = 0.48209$. This corresponds to 25.738 degrees lattice. So that's the critical threshold.

Mode $m_1 = n/2,\ m_2 = 0$

$$M_{11} = \sum_{j_1=1}^{n_1-1} \sum_{j_2=0}^{n_2-1} G_{xx}(x_j, y_j)\left(\exp\{\pi i j_1\} - 1\right), \quad x_j = \frac{L}{n}\left(j_1 + \frac{j_2}{2}\right) \bmod L, \quad y_j = \frac{H}{n}\frac{j_2}{2}.$$

Split the sum: $M_{11} = I_1 + I_2$, where

$$I_1 = -\frac{2\pi}{L^2} \sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2-1} \sum_{q=1}^{\infty} q \cos\left(2\pi q \frac{\left(j_1 + \frac{j_2}{2}\right)}{n}\right) \frac{\cosh\left(\left(\frac{H}{n}\frac{j_2}{2} - H/2\right)\frac{2\pi}{L} q\right)}{\sinh\left(\frac{2\pi}{L} q H/2\right)} \left(\exp\{\pi i j_1\} - 1\right)$$

$$I_2 = \sum_{j_1=1}^{n-1} \left\{ \frac{1}{HL} + \frac{2\pi}{H^2} \sum_{q=1}^{\infty} q \frac{\cosh\left(\left(\frac{L}{n} j_1 - L/2\right)\frac{2\pi}{H} q\right)}{\sinh\left(\frac{2\pi}{H} q L/2\right)} \right\} \left(\exp\{\pi i j_1\} - 1\right)$$

For I_1 we sum over j_1 first:

$$I_1 \sim n^2 \frac{2\pi}{L^2} \sum_{j_2=1}^{\infty} \sum_{Q=1}^{\infty} Q \exp\left(-H j_2 \frac{\pi}{2L} Q\right) \cos\left(\pi Q \left(1 + \frac{j_2}{2}\right)\right);$$

For I_2 we do resummation (EWALD) tricks:

$$I_2 \sim -\frac{n}{HL} - \frac{4\pi}{H^2}\sum_{k=0}^{\hat{n}-1}\sum_{q=1}^{\infty} q\frac{\cosh\left(aq\left(1-\frac{2k}{\hat{n}}-\frac{1}{\hat{n}}\right)\right)}{\sinh\left(aq\right)}$$

$$.... \sim -\frac{\pi n^2}{4L^2}$$

Summary:

$$M_{11} \sim -\frac{\pi n^2}{4L^2} + n^2\frac{2\pi}{L^2}\sum_{j_2=1}^{\infty}\sum_{Q=1}^{\infty} Q\exp\left(-Hj_2\frac{\pi}{2L}Q\right)\cos\left(\pi Q\left(1+\frac{j_2}{2}\right)\right)$$

Similar for $M_{22},\ M_{11}$.

Competition instabilities for Schnakenberg model

- There are 4N eigenvalues in total
  - 2N “small” eigenvalues from linearization of the ODE
  - 2N “large” eigenvalues whose crossing triggers competition instability
  - Small eigenvalues are triggered by e.g. changing domain shape
  - Large eigenvalues are triggered by decreasing feed rate A.

- **Main result:** Define

$$A_m := \frac{1}{\log \varepsilon^{-1}} \frac{N}{|\Omega|} \left(2\pi \int w^2 \right)^{1/2} \left(1 + \frac{2\pi}{\log \varepsilon^{-1}} \tilde{\Upsilon}(m) \right)^{-1/2} \tag{20}$$

$$\tilde{\Upsilon}(m) = \sum_{l \neq 0} \exp \left\{ 2\pi i \left(\frac{m_1}{n_1} l_1 + \frac{m_2}{n_2} l_2 \right) \right\} G(vl) + R_0. \tag{21}$$

Here, R_0 is the regular part of G, given by

$$R_0 = \lim_{x \to 0} \left(G(x) + \frac{1}{2\pi} \log |x| \right) \tag{22}$$

$$= \frac{R}{12L} - \frac{1}{2\pi} \log \left(\frac{2\pi}{L} \right) - \frac{1}{\pi} \sum_{n=1}^{\infty} \log \left(1 - \exp \left(-\frac{2\pi R}{L} n \right) \right). \tag{23}$$

For each choice of $m \in \mathbb{Z}_{n_1} \times Z_{n_2}$, there is a bifurcation (zero eigenvalue) when $A \sim A_m$, and an unstable eigenvalue if $A < A_m$.

- **Corrollary.** Let

$$A_c = \max_{m \in \mathbb{Z}_{n_1} \times Z_{n_2}} (A_m)\,; \tag{24}$$

Competition instability is triggered when A is decreased below A_c. The shape of instability is given by the mode $m = (m_1, m_2)$ which minimizes $\tilde{\Upsilon}(m)$.

Example

- Take $L = H = 2, \varepsilon = 0.024$, $A = 90$. Then Turing instability results in a regular lattice of $N = 24$ spots. Movie

- ***Theory:*** $A_c = 34.6$; mode $m = (12, 0)$. ***Numerics***: $A \approx 39$,mode $m = (8, 0)$ is observed! Movie
  - $\tilde{\Upsilon}(12, 0) = -0.2218$; $\tilde{\Upsilon}(8, 0) = -0.2211$; only 0.3% difference between the modes

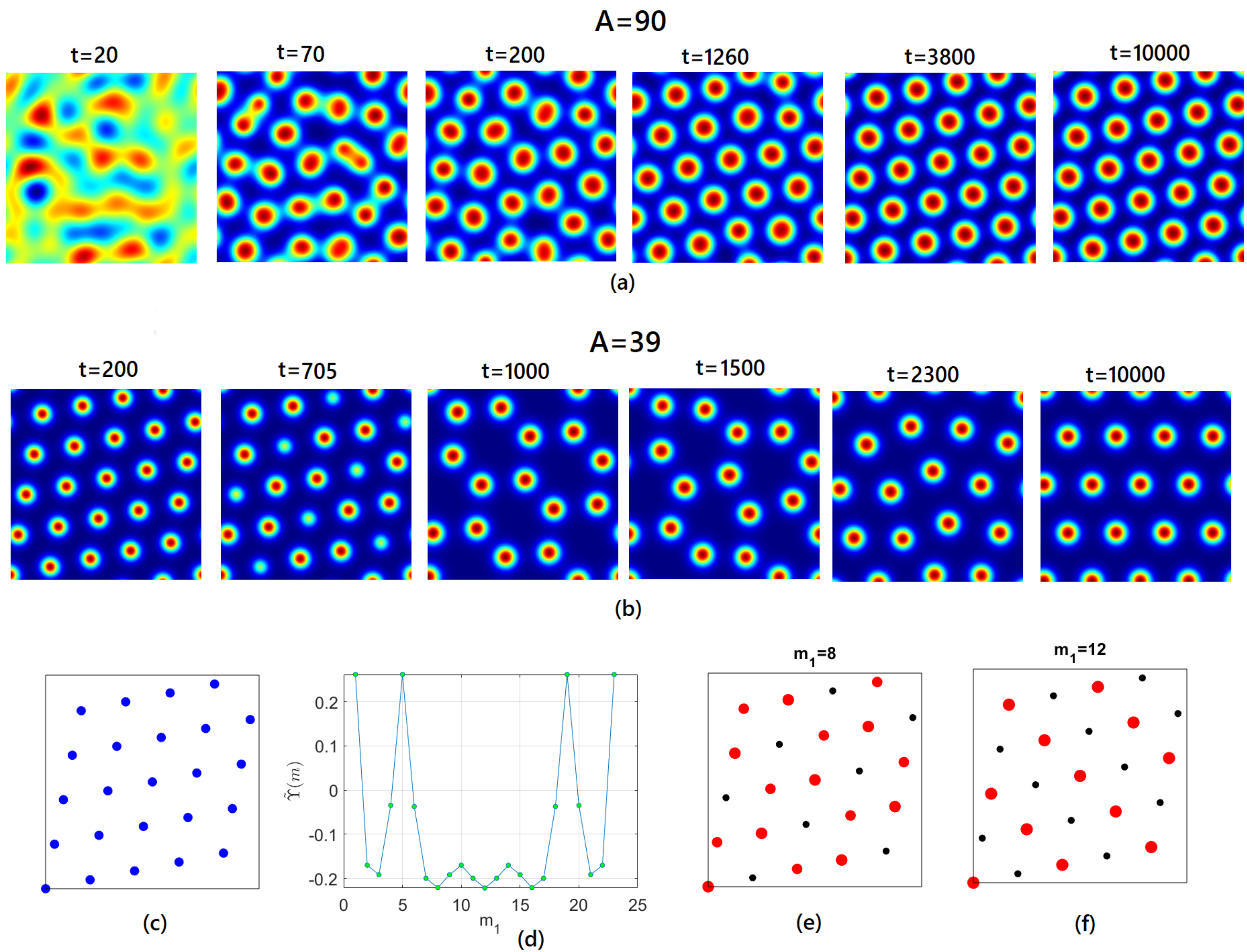
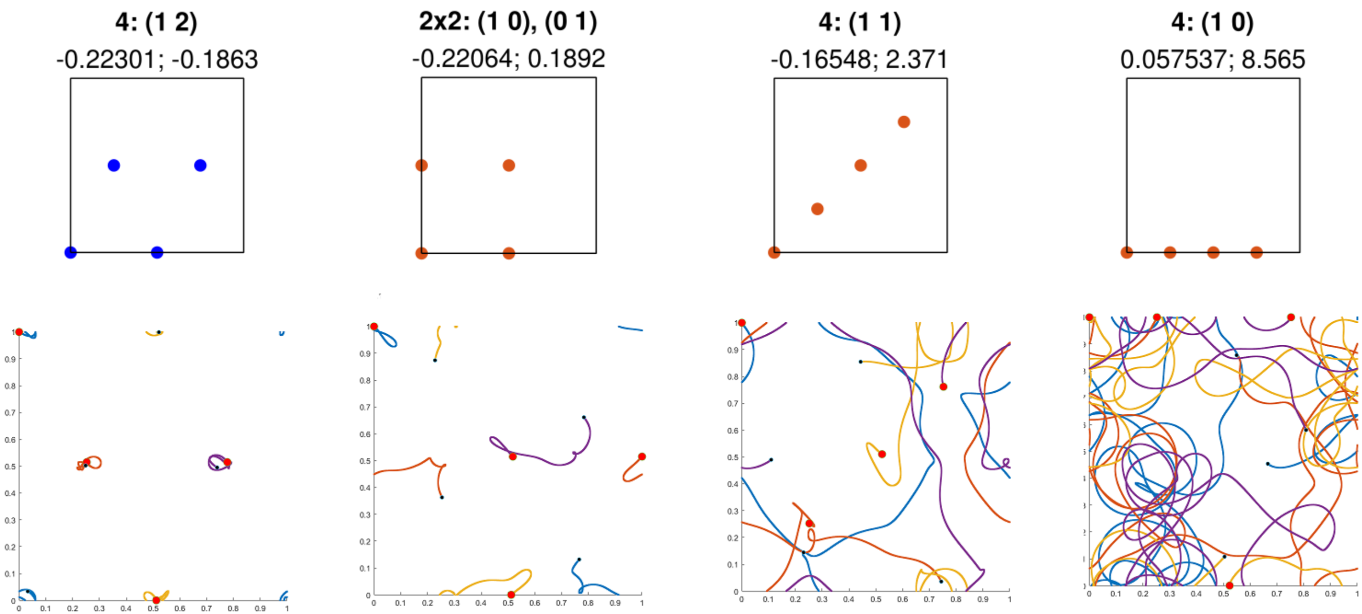


Figure 1: (a) Simulation of (**??**) starting with random initial conditions. The parameter values are $\Omega = (0, 2) \times (0, 2)$; $A = 90$, $\varepsilon = 0.04$. After some complicated

Experiment: point vortices on periodic rectangle

$$
\begin{aligned}
iy_k' &= \sum_{j \neq k} G_1(x_j - x_k, y_j - y_k) \\
-ix_k' &= \sum_{j \neq k} G_2(x_j - x_k, y_j - y_k).
\end{aligned}
$$

$N{=}4$



Open questions/future work

- Numerical optimization suggests that stable regular lattices are often ***global minimizers.*** See fig for $N \leq 30$. Can this be proven for ***some*** N and/or some aspect ratio? Maybe for the perfect hexagonal lattice ($L/H = \sqrt{3}$, $N = 2n^2$)?
- There is no stable lattice on a square for $N = 6, 7, 13, 21, 26, 31, 37, 41, 44, 51, 55, 65, 71, 89$. What about $N > 100$? Are there infinitely many N for which there is no stable regular lattice?
  - **Conjecture:** there will always be a regular lattice for sufficiently large N...
- Complex bifurcation structure result in many novel patterns such as "bended lattice" etc. Example: changing aspect ratio, N=23
- Rigorously prove stability of hexagonal pattern (i.e. do ***all*** modes)...
- References

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