Turing Patterns for Nonlocal Diffusive Systems

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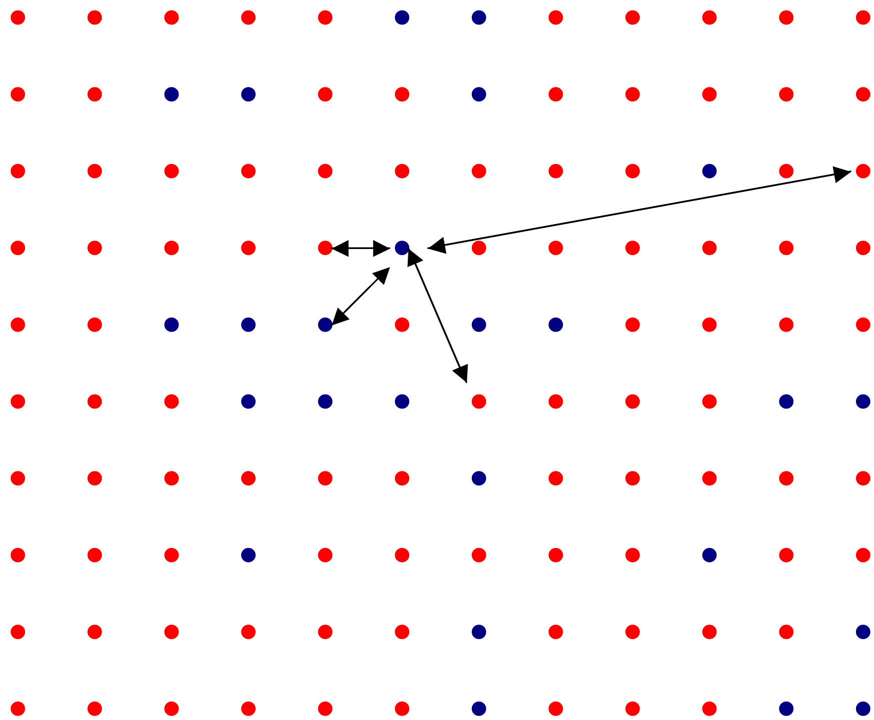


FIGURE 1, LATTICE

A material occupying an n-dimensional lattice Λ

Sites occupied by atoms of 'spin' A or B.
Occupancy of type A at $r \in \Lambda$ is $a(r) \in [0, 1]$.

The STATE of the material is the function $a : \Lambda \to [0, 1]$, which also evolves in time.

"We shall obtain a complete solution of the problem ... if we can express *the free energy* at each point as a function of the density at that point and of the differences of density in the neighboring phases, out to a distance limited by the range over which the molecular forces act"
J.D. van der Waals, 1893

The HELMHOLTZ FREE ENERGY of a state:

$$E = H - TS$$

where H = interaction energy, T = absolute temperature, and S = total entropy of mixing.

$$H(a) \equiv -\frac{1}{2} \sum_{r,r' \in \Lambda} \Big[J^{AA}(r-r')a(r)a(r') +$$

$$J^{BB}(r-r')(1-a(r))(1-a(r')) +$$

$$J^{AB}(r-r')(a(r)(1-a(r')) + a(r')(1-a(r))) \Big].$$

The J's (interaction coeff's) are symmetric, translation-invariant, anisotropic. Rearranging:

$$H = \frac{1}{4} \sum_{r,r' \in \Lambda} J(r-r')(a(r)-a(r'))^2 -$$

$$D \frac{1}{2} \sum_{r \in \Lambda} (a(r)^2 - a(r)) + d \sum_{r \in \Lambda} a(r) + \text{const.}$$

where $J(r) = J^{AA}(r) + J^{BB}(r) - 2J^{AB}(r)$, $D = \sum J(r)$, and $d = \sum (J^{BB}(r) - J^{AA}(r))/2$.

At site r the entropy $s(a(r))$ for aN particles in N identical sites is given by

$$e^{Ns/K} = \frac{N!}{(aN)!(N-aN)!}$$

where K is Boltzman's constant.

Hence,

$$s(a) \simeq -K[a \ln a + (1-a)\ln(1-a)].$$

The total entropy, $S(a) = \sum_{r\in\Lambda} s(a(r))$ and so

$$E(a) = H - TS =$$

$$\frac{1}{4}\sum_{r,r'\in\Lambda} J(r-r')(a(r)-a(r'))^2$$

$$+\sum_{r\in\Lambda}\Big[KT\{a(r)\ln a(r) + (1-a(r))\ln(1-a(r))\}$$

$$-D(a(r)^2 - a(r)) + da(r)\Big].$$

There is a critical temperature T_c such that for $T \geq T_c$ the term $[\,\cdots\,]$ is strictly convex and so there is a unique homogeneous state which minimizes $E(a)$, while for $T < T_c$, this term has two local minima and so two distinct a-states (say $\alpha < \beta$) give spatially homogeneous local minimizers of E. This is the origin of phase transition in spin systems (e.g. ferromagnets.)

We will fix $T < T_c$. Take continuum limit. This gives the free energy in the isothermal case of the form

$$E(u) = \frac{1}{4} \iint J(x-y)(u(x)-u(y))^2 dxdy + \int F(u)dx,$$

where F is a double well function, having minima at ± 1 (after changing variables), and J is assumed to be integrable with positive integral and with $J(-x) = J(x)$. Compare with G-L functional:
$(u(x) - u(y)) \simeq (x - y) \cdot \nabla u(x)$.

IMPORTANT: For several results we de not require that J be nonnegative.

A fundamental principle: A material structure evolves in such a way that its FREE ENERGY decreases as quickly as possible. The spatial function u will evolve in such a way that $E(u)$ decreases, and does so optimally in some sense. This suggests the evolution law

$$\frac{\partial u}{\partial t} = -\,\mathrm{grad} E(u) \quad (*)$$

grad $E(u) \in X^*$ is defined by

$$< \mathrm{grad}\ E(u), v >= \frac{d}{dh} E(u + hv)|_{h=0}.$$

If $X = L^2$ then (*) becomes

$$\frac{\partial u}{\partial t} = J * u - Du - F'(u) \quad \text{(NAC)}$$

where $*$ is convolution and $D = \int J$ is assumed positive.

The operator

$$Lu(x) \equiv J * u - u \int_\Omega J(x-y)dy$$
$$\equiv \int_\Omega J(x-y)u(y)dy - u(x) \int_\Omega J(x-y)dy$$

has some features in common with the Laplacian.
For example, $L1 = 0$, and if $J \geq 0$ then L is a self adjoint non-positive operator and a maximum principle holds.

It appears in equations of materials science, dispersion of vegetation, mutation, neuroscience and various jump processes.

It is diffusion-like but it is a bounded operator, unlike the Lapacian.

We assume

$J \in C_c^1$, $J \gneq 0$, $J(z) = \tilde{J}(|z|)$, and $\tilde{J}'(|z|) \leq 0$.

We can consider the system

$$\frac{du}{dt} = d_u L u + f(u, v)$$

$$\frac{dv}{dt} = d_v L v + g(u, v)$$

and ask if Turing patterns emerge from a homogeneous steady state which is stable under the kinetics, i.e., that state becomes unstable when 'diffusion' is added with very different coefficients.

With the usual requirements on a homogeneous steady state (p, q), one is directed to consider the spectrum of

$$L\mathrm{diag}(d_u, d_v) + \mathrm{Jac}(f, g)(p, q).$$

First we need the spectrum of L, but this is not easy to find for a general kernel and a general domain.

In the case on $\Omega = \mathbb{R}^n$

$$L_0 u(x) \equiv \int_{\mathbb{R}^n} J(x-y)u(y)dy - u(x)$$

where $\int J = 1$, if we rescale and consider

$$J_\varepsilon(x) \equiv \varepsilon^{-n} J(x/\varepsilon)$$

and write

$$L_\varepsilon u(x) \equiv \frac{1}{\varepsilon^2}[J_\varepsilon * u - u]$$

Then one might imagine that as $\varepsilon \to 0$, $L_\varepsilon \to \Delta$.

Clearly this cannot be true since the difference between the two operators is an unbounded operator. However,

Lemma (B-Chen-Chmaj, '03, '05)
For all $\phi \in H^2(\mathbb{R})$

$$L_\varepsilon \phi \to c_J \Delta\phi \ \textit{as}\ \varepsilon \to 0,$$

where $c_J = \int |z|^2 J(z)/2$.

Similarly, on a bounded domain $\Omega \subset \mathbb{R}^n$ with

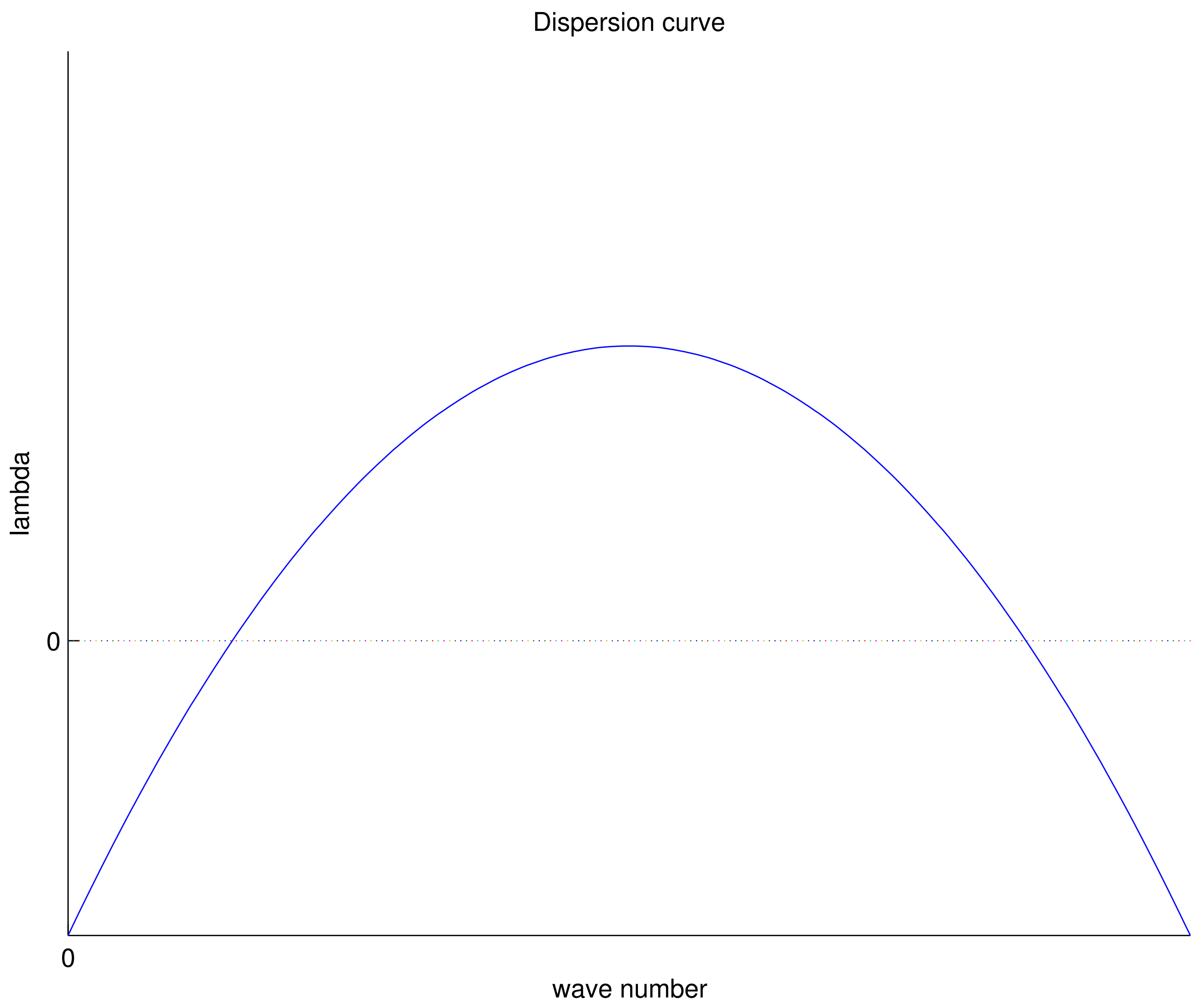
$$L_\varepsilon u(x) \equiv \frac{1}{\varepsilon^2} \int_\Omega J_\varepsilon(x-y)(u(y)-u(x))dy$$

the same result was proved by Cortazar, et al in 2008. In this case Δ is the Neumann Laplacian.

Notice that this is pointwise (not operator) convergence and so it is a nontrivial question to ask if the spectrum of L_ε is close to that of $c_J \Delta^N$.

Actually, it is a trivial question, since the answer is NO! (A bounded set is not close to an unbounded set)

HOWEVER, recall the essentials of the Turing instability:



What we need is for each $M > 0$

$$\sigma(L_\varepsilon) \cap [-M, 0] \to \sigma(c_J \Delta) \cap [-M, 0] \text{ as } \varepsilon \to 0.$$

Lemma 1 *Given a compact subset* $\Theta \subset \rho(c_J \Delta^N)$, *there exists* $\epsilon_\Theta > 0$ *such that* $\Theta \subset \rho(L_\epsilon)$ *if* $\epsilon \leq \epsilon_\Theta$.

The proof is by contradiction: Assume there is a sequence $\varepsilon_k \to 0$ and $\lambda_k \in \Theta$ so that for each k, there is a sequence $\{v_k^j\}_j \subset 1^\perp$ for which

$$\|(L_{\epsilon_k} - \lambda_k I) v_k^j\| \to 0 \text{ as } j \to \infty.$$

Do some work to get $v_k^j \to w_k$ as $j \to \infty$, obtaining

$$\|(L_{\epsilon_k} - \lambda_k I) w_k\| \leq \frac{1}{k}.$$

Now show convergence of $\{w_k\}$ and use $L_\varepsilon \to c_J \Delta$ and get a contradiction.

Proposition 0.1 *Assume that* $\Theta \subset \rho(L_\epsilon) \cap \rho(c_J \Delta^N)$ *for all* $\epsilon \le \epsilon_\Theta$*, where* $\Theta \subset \mathbb{C}$ *is compact. Then there exist* $\theta > 0$ *and* $\bar{\epsilon}_\Theta > 0$ *such that*

$$\|(\lambda I - L_\epsilon)^{-1}\| \le \theta \quad \text{for all} \quad \lambda \in \Theta, \ \ \epsilon \le \bar{\epsilon}_\Theta.$$

Furthermore, $(\lambda I - L_\epsilon)^{-1} u \to (\lambda I - c_J \Delta^N)^{-1} u$ *strongly in* $L^2(\Omega)$ *as* $\epsilon \to 0$*, for each* $u \in L^2(\Omega)$*, uniformly in* $\lambda \in \Theta$*.*

Theorem 1 *Assume that* $\mu \in \sigma(c_J \Delta^N)$ *and let* $B_\delta = \{\lambda \in \mathbb{C} \mid |\lambda - \mu| \le \delta\}$ *with* $\delta > 0$ *so small that* $B_\delta \cap \sigma(c_J \Delta^N) = \{\mu\}$*. Then there exists* $\epsilon_\delta > 0$ *such that* $B_\delta \cap \sigma(L_\epsilon) \ne \varnothing$ *and* $B_\delta \cap \sigma(L_\epsilon) \subset \sigma_d(L_\epsilon)$ *for all* $\epsilon \le \epsilon_\delta$*. Furthermore, if* $\dim \ker(\mu I - c_J \Delta^N) = m$ *then* $L_\epsilon (\epsilon \le \epsilon_\delta)$ *has at most* m *isolated eigenvalues* $\mu_j^\epsilon \in B_\delta (1 \le j \le m)$ *with total multiplicity equal to* m*.*

The proof uses ideas from Kato, including the contour integral representation of spectral projection operators, the proposition above, and the convergence of the nonlocal operator to the Laplacian, among other things.

TURING PATTERNS

Consider the following system for $d > 1$

$$\begin{cases} \dfrac{\partial u}{\partial t} = \gamma L_\varepsilon u + f(u,v), \\ \dfrac{\partial v}{\partial t} = d\gamma L_\varepsilon v + g(u,v) \qquad \text{in} \quad \Omega \times [0,\infty). \end{cases} \tag{1}$$

We assume that $(p,q)^T \in \mathbb{R}^2$ is a stable homogeneous equilibrium of the kinetic system, that is, $f(p,q) = g(p,q) = 0$ and $\mathrm{Jac}(f,g)(p,q)$ has two eigenvalues with negative real parts. We also assume that $f, g \in C^{2+\theta}(\mathbb{R}^2, \mathbb{R})$ for some $\theta \in (0,1)$. $\Omega \subset \mathbb{R}^n$ is a bounded domain with smooth boundary, and $\gamma > 0$ is a spatial scale factor. Linearizing around $(p,q)^T$ gives

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}\begin{pmatrix} \gamma L_\epsilon u \\ \gamma L_\epsilon v \end{pmatrix} + \begin{pmatrix} f_u(p,q) & f_v(p,q) \\ g_u(p,q) & g_v(p,q) \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}. \tag{2}$$

Let

$$A_\epsilon = \gamma D L_\epsilon + B \tag{3}$$

where

$$D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}, \qquad B = \begin{pmatrix} f_u(p,q) & f_v(p,q) \\ g_u(p,q) & g_v(p,q) \end{pmatrix}.$$

Following Sander and Wanner (JDE '03) we impose the Turing conditions for local diffusion:

(H1) $f_u|_{(p,q)} > 0$, $\text{tr}B = (f_u + g_v)|_{(p,q)} < 0$.

(H2) $\det B = (f_u g_v - f_v g_u)|_{(p,q)} > 0$.

(H3) $(f_u + g_v)^2 - 4(f_u g_v - f_v g_u)|_{(p,q)} > 0$.

(H4) $(df_u + g_v)|_{(p,q)} > 0$.

(H5) $(df_u + g_v)^2 - 4d(f_u g_v - f_v g_u)|_{(p,q)} > 0$.

Set

$$C(s) = B + sD.$$

$$\det[C(s) - \lambda I] = \lambda^2 - b(s)\lambda + c(s),$$

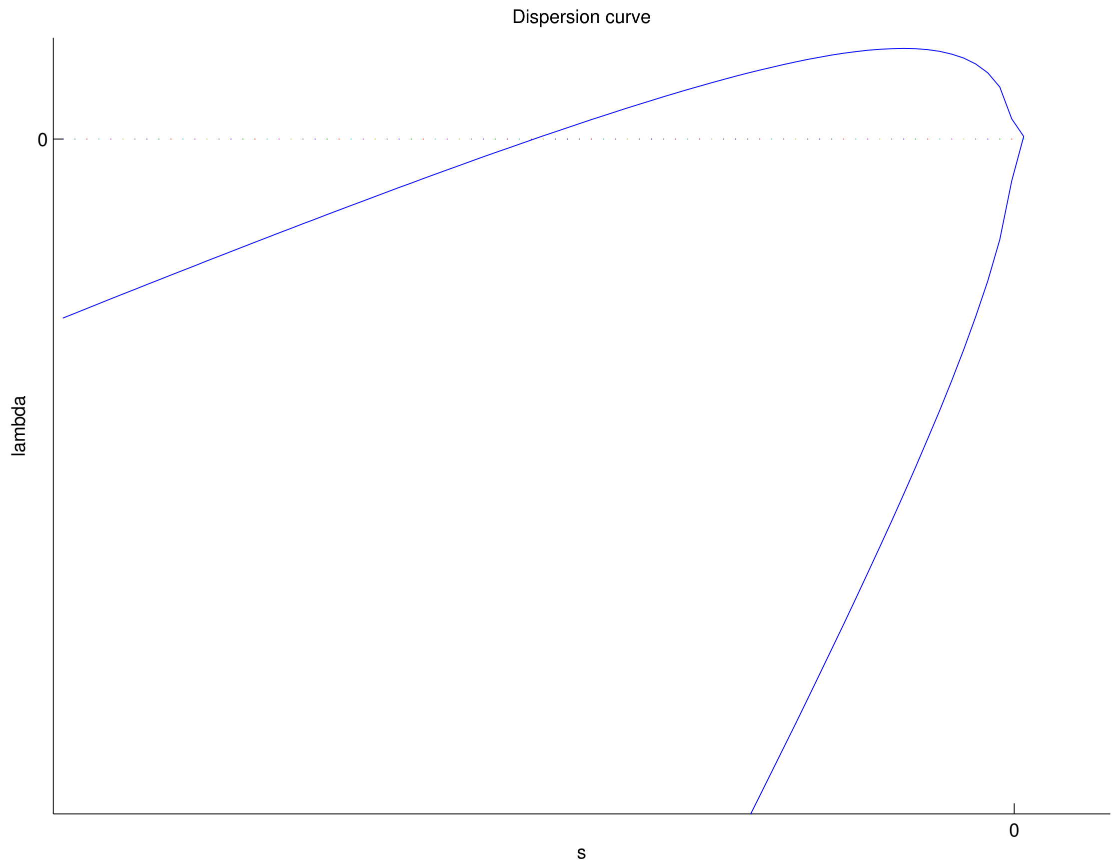
where $b(s) = (f_u + g_v)|_{(p,q)} + s(1 + d)$,
$c(s) = (f_u g_v - f_v g_u)|_{(p,q)} + s(df_u + g_v)|_{(p,q)} + ds^2$.

$s \to \lambda(s)$ such that $\det C(s) = 0$ has two real branches $\lambda^-(s) < \lambda^+(s)$ for all $s \le 0$.

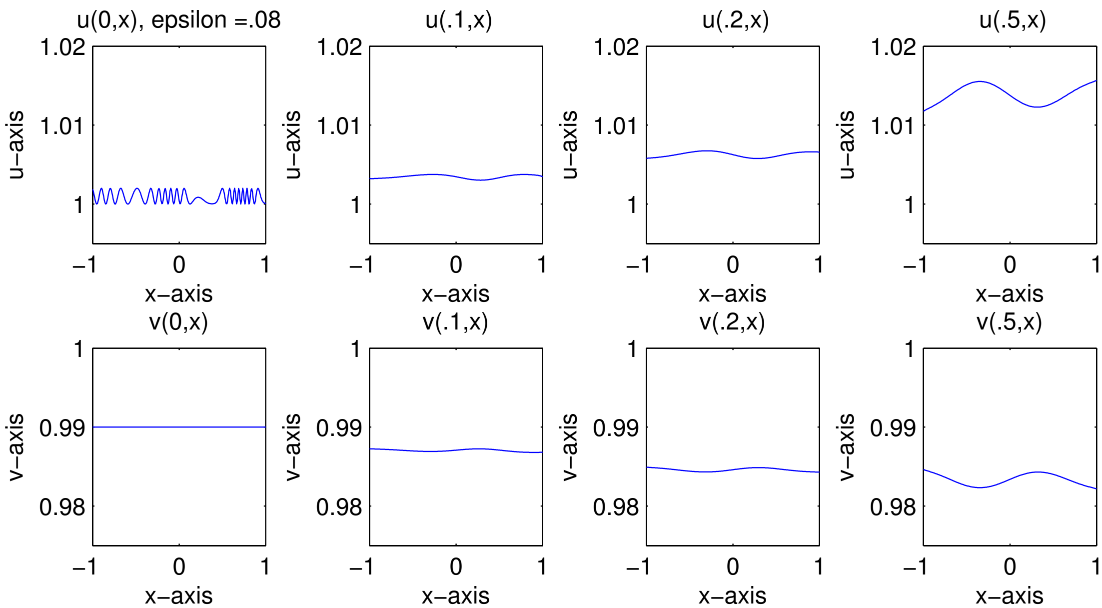
$\lambda^-(s)$ is strictly increasing

$\lambda^+(0) < 0$, $\lambda^+(s)$ has a unique maximum $\lambda^+_{\max}$ attained at some $s_{\max} < 0$.

Note that s stands for the spectral parameter from γL_ε and so $s \le 0$ is what concerns us.


Dispersion curve
0
lambda
0
s

For the Schnakenberg system with nonlocal diffusion:



Other results

Sander-Tatum (ejde 2013) have results for local/nonlocal systems. They assume Ω is a rectangle in 2, 3, or 4 dimensions and that J is given as a Fourier series. There is some scaling but I have not understood it:

$\varepsilon^\theta J(x) \to K(x)$ as $\varepsilon \to 0$ but there does not seem to be a description of how J depends on ε, otherwise. Here $\theta < 1$ and so this is certainly not our situation and it seems that effectively, J becomes relatively negligible as $\varepsilon \to 0$.

Hutt and Atay: Spatio-temporal patterns in systems with space-dependent time delays. Related to earlier work of Ermentrout, et al.

Viana, Silva, Lopes: One dimensional chain of oscillators.