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Meeting of Chemical Wave Fronts Creates Chaos

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Abstract: We consider systems of reaction–diffusion equations. We describe a new effect in the wave interaction for these systems: the collision of several travelling fronts may induce chaos or periodic oscillations. This effect depends on the initial locations of the travelling fronts: For some initial positions chaos occurs and for others it does not. In a space-homogeneous system, we need at least three fronts to create time-periodic behaviour, while to create chaos, we should have four fronts. We also provide a short review of previously known results, and different known mechanisms of chaos generation for reaction–diffusion systems. Our results can be used for pattern coding, in particular, for morphogenesis.

Keywords: reaction–diffusion systems; waves; chaos

MSC: 35K57; 37D45

1. Introduction

In this paper, we prove the existence of a new effect in the interaction of wave fronts for reaction–diffusion systems. These systems have important applications in biology, ecology, chemistry (combustion), and physics (see, for example, [1,2]). They exhibit travelling front propagation, an effect important in ecology, when one species replaces another. This could be a result of climate change or species invasive properties. The first existence of such fronts was proved mathematically in seminal works [3,4] for reaction–diffusion equations (see [2] for more detail). Recall the travelling wave is a solution of the form $U(x - Vt)$, where V is a constant speed. Great attention was devoted to this domain after the remarkable paper [5]. The results of this work allow us to understand the large-time behaviour of solutions for a large class of reaction–diffusion equations, in particular, what can happen if two travelling waves meet. Although we are not capable of describing the collision process in detail, the result will always be either a new travelling wave or a constant solution $U(x,t) \equiv const$. An exhaustive survey of these classical results can be found in [2].

From an application point of view, systems of reaction–diffusion equations are of much greater interest; however, up to now there is an absence of general analytical results on the existence and interaction of travelling waves, with the exception of some particular classes of systems. For example, the results on the existence of the waves can be extended to the case of so-called monotone reaction–diffusion systems. An n-component system with a reaction part $f_i(u)$, where $u = (u_1, \dots, u_n)$ and f_i are smooth functions, is called monotone if $\frac{\partial f_i}{\partial u_j} \geq 0$ for all $i \neq j$. The reason why monotone systems can be investigated successfully and the results are similar to the simplest case of one equation ($n = 1$) can be explained as follows. In both cases, the corresponding dynamical systems generate monotone semiflows S^t, $t > 0$, in appropriate phase function spaces $\mathbb{H}$. A semiflow defined on the partially ordered Banach space $\mathbb{H}$ is monotone if it conserves a partial order $>>$ in that space. The general theory of monotone dynamical systems was developed first in the seminal works of M. Hirsch's (see [6] for an overview).

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For monotone reaction–diffusion systems the partial order can be defined as so: $u >> v$ if $u_i > v_i$ for each i. For chemical kinetics, the monotone dynamics means the following. Let $u_i(x,t)$, $i = 1,\ldots,n$ be concentrations of reagents participating in chemical kinetics. Let us consider two sets of concentrations, u and v, which both evolve according to given monotone chemical kinetics. Then, if all initial concentrations $u_i(x,0)$ are more than the corresponding initial v concentrations, $u_i(x,0) \geq v_i(x,0)$ for each i and $x \in \Omega$, where the domain Ω_i is a chemical reactor, this relation is conserved for all $t > 0$: $u_i(x,t) \geq v_i(x,t)$ for all $i, x, t > 0$. Roughly speaking, larger input concentrations produce larger output concentrations at each time moment.

However, unfortunately the reaction–diffusion systems that are most interesting for applications are not monotone. What could happen in the non-monotonic case? Some investigations and results, obtained using mainly asymptotical and numerical methods, have shed light on this problem. The question of the existence of chaotic regimes in chemistry received great attention in the 1980s–1990s. First, one can note that if a reactor is well stirred and we consider a spatially homogeneous state, then we can take a system of reaction–diffusion under zero Neumann boundary conditions, where the reaction part generates chaotic behaviour (clearly, in this case we need at least three reagents). It is easy to show then that if diffusion coefficients are sufficiently large, this dynamical chaos is stable under space perturbations. This case, however, is not interesting for us since it it just the usual dynamical chaos, where diffusion effects play no role. Moreover, in this case we do not have any wave phenomena. In the space-homogeneous case, the first two beautiful ideas were proposed in Kuramoto's book [7]. The first one can be outlined as follows. Suppose that the reaction part generates a limit cycle, i.e., we are dealing with a chemical oscillator. If diffusion is absent (the diffusion coefficients are equal to zero), then we have an infinite set of oscillators located at points x of the reactor. All oscillators oscillate the same way, but each of them has its own phase $\phi(x)$ depending on the point x. For small diffusion coefficients one can develop an asymptotic approach, which has a transparent physical sense: it describes a weak interaction between oscillators via diffusion. The phase becomes a function of x and time t. One can show that the phase evolution is governed by the famous Burgers equation, which can be linearized and reduced to the heat transfer equation. If the heat conduction coefficient is positive, all the solutions of the Burgers equation are time convergent. Physically, this means that all oscillators are synchronized in the limit of large times. If the heat conduction coefficient is negative, we have an exponential instability of solutions of the Burgers equation for the phase. This can be interpreted as chaos (turbulence) describing the desynchronization of the oscillators. Such an effect arises for special reaction parts and, moreover, the diffusion coefficients should be different. It is not easy to justify these asymptotical results using rigorous methods (however, if we replace a space-continuous model with a discrete one, i.e., consider oscillators on a lattice, then it can be achieved using standard methods). Moreover, we do not have wave phenomena here. Nonetheless, this Kuramoto model can be extended to describe moving chaos that captures more and more new territories.

The second idea from [7] describes chemical wave fronts unstable in space, and it was pioneered independently by Sivashinsky [8] for combustion and other authors for fluid dynamics [9,10]. This instability problem, leading to the intriguing Kuramoto–Sivashinsky equation, is studied in many works, and we do not consider it in this paper.

A number of non-trivial wave effects induced by diffusion in chemistry were found in [11,12] using numerical simulations. In these works, simple cubic autocatalytic models are investigated. It is shown that complex dynamics, induced initially by the propagation of a constant-velocity constant-form reaction wave, is possible. The chaotic nature of this wave can be confirmed by numerical methods (but it is hard to justify it using analytical approaches).

In [13], the wave solutions are found using numerical simulations for a disease propagation model, which has the form of a two-component reaction–diffusion system. The results in [13] show that spatio-temporal chaos can be generated by waves. Ref. [14] also concerns a two-component reaction–diffusion system, describing a predator–prey model taking into account species migration. It is shown that there are possible patterns corresponding to

spatio-temporal chaos. These patterns appear inside a space subdomain and then the chaotic pattern invades all the area.

In our work, we propose a model, which, in contrast to those mentioned above, can be studied using rigorous methods, and moreover, it permits us to describe wave collisions. The main result can be outlined as follows. There are possible interesting phenomena in the collisions of wave fronts. In contrast to one-component and monotone cases, in the general situation, when travelling wave fronts meet they are capable of producing chaotic or periodic solutions. The result of the collision of waves depends on their initial positions. We show that in the spatially homogeneous case time periodical solutions are possible for $n > 2$ and chaotic solutions for $n > 3$. The result of the waves meeting are so-called generalised travelling waves (GTWs), earlier studied in [15]. GTWs have solutions of the form

$$u = U(x, q(t)), \quad u_i = U_i(x - q_i(t)),$$

where $U(x)$ is a function and $q_i(t)$ satisfies the system of ordinary differential equations

$$\frac{dq_i}{dt} = Q_i(q), \tag{1}$$

where $q = (q_1, \ldots, q_n)$, and Q is a smooth vector field. This means that the solution is a family of travelling fronts where each front moves with the speed $Q_i(q)$. However, the fronts are not independent: each component, in general, depends on each other.

Let us outline the physical mechanism beyond the complicated dynamics. This mechanism is fundamental and it is connected with spontaneous symmetry breaking. To start, let us consider the simplest case of a reaction–diffusion equation. We consider the scalar, time-dependent Ginzburg–Landau (TDGL) equation. This equation describes the dynamics in a bistable medium where there are two stable thermodynamically equivalent states. This basic equation belongs to a family of canonical equations which govern the dynamics of condensed matter at a critical point. The scalar Ginzburg–Landau equation corresponds to the simplest case, where the system mass is not conserved and the order parameter is a scalar [16,17]. The TDGL equation is well studied and describes interesting effects, in particular, there exist kink solutions and solutions describing kink chains [18]. The TDGL equation reads

$$u_t = \frac{1}{2}u_{xx} + u - u^3. \tag{2}$$

This equation describes a dissipative process. In fact, the Ginzburg–Landau energy, which is

$$E[u(\cdot,\cdot)] = \int_{-\infty}^{\infty} \left(u_x^2 + (1-u^2)^2\right) dx$$

decreases along trajectories defined by (2). This energy is the sum of two contributions, the Landau term $\int (1-u^2)^2 dx$ and the Ginzburg gradient term $\int u_x^2 dx$. The Landau term has two absolute minima $u_\pm \equiv \pm 1$, which correspond to two stable phases minimizing the free energy of a bistable medium. There exist, however, more non-trivial solutions (kinks) corresponding to transitions from one phase to another:

$$u_{kink} = \tanh(x - q),$$

where q defines a kink location. The kink is a standing wave because the system is bistable and both phases $u_\pm$ are energetically equivalent. We have a family of kink solutions parameterized by q. The existence of such a family, which can be considered as a one-dimensional manifold embedded in the infinite-dimensional phase space, is connected with the translation invariance (symmetry) of our bistable medium: all positions q are equivalent. Interesting solutions of the TDGL are studied in [18]. They describe kink chains where the kinks are separated by long intervals. The kinks move very slowly due to an exponentially weakening interaction between the closest kinks. It is very difficult to

detect this slow evolution using numerical methods [18]. In this paper, we use an approach similar to in [18].

Even more interesting phenomena arise if we consider a more complicated model:

$$u_t = \frac{1}{2}u_{xx} + u - u^3 + \lambda g(u, x), \tag{3}$$

where $\lambda > 0$ is a small parameter, g can be interpreted as a small perturbation violating the phase symmetry. This weak perturbation breaks the bistability symmetry. In this case, the equilibrium spatially homogeneous system states $u_\pm$ become energetically non-equivalent. This perturbation g causes two effects. The first effect is that the shape of the kink experiences a slight deformation and the second effect is that the kink begins to move slowly, i.e., q depends on t. For the kink coordinates q we obtain

$$dq/dt = \lambda Q(q, g(\cdot, \cdot)), \tag{4}$$

where Q is a linear functional of the perturbation g:

$$Q = C^{-1} \int_{-\infty}^{\infty} g(u_{kink}(x, q), x)\tilde{\mathcal{U}}(x, q)dx,$$

Here,

$$\tilde{\mathcal{U}}(x, q) = \frac{\partial u_{kink}(x, q)}{\partial q}$$

denotes the so-called Goldstone's mode, which appears in all physical models with symmetry, and

$$C = -\int_{-\infty}^{\infty} \tilde{\mathcal{U}}(x, q)^2 dx.$$

The expression for Q can be obtained in different ways. The most natural asymptotic derivation (although non-rigorous) of (4) can be achieved using energetic arguments (see Appendix B). The rigorous justification has been presented in many works (see, for example, [18]). An asymptotic approach was first developed in [19].

Furthermore, let us consider the n independent instances of Equation (2) for unknown $u_i(x, t)$, $i = 1, \ldots, n$, where each equation contains a small perturbation $g_i(u_1, \ldots, u_n)$. Then, using the same arguments and methods as for a single equation we can show that there is a set of kink solutions $\tanh(x - q_i(t))$ where each kink moves according to

$$dq_i/dt = \lambda Q_i(q, g_i(\cdot, \cdot)), \quad q = (q_1, \ldots, q_n). \tag{5}$$

Using different g_i we can obtain a rich family of different Q_i that allows us to find complicated effects in multi-component kink collisions.

The construction has a transparent interpretation. In a multi-component system where separate components interact weakly, there arises a weak interaction between kinks. When the kinks become closer to each other, this interaction leads to the formation of a complicated connected state of kinks. This connected state can evolve chaotically or periodically in time. However, the chaos emerges when these kinks come closer together. If at initial moment $t = 0$ the wave fronts are far from each other, then the interaction is absent and we observe a collection of usual travelling fronts which move independently. The complicated time behaviour and oscillations arise when the fronts are close enough. This mechanism of chaos onset is illustrated in Figure 2.

We think that such behaviour is also possible in systems other than reaction–diffusion systems, because the effect is quite general and admits an energetic interpretation (see Appendix B).

Note that numerical simulations show that chaotic waves exist for realistic models of population dynamics; see [14]. They extend our possibilities in pattern formation and can be applied for pattern coding and morphogenesis problems; see [20,21]. A key difference

between chaotic waves and usual travelling fronts can be understood if we consider the somitogenesis problem [22–24]. Somitogenesis is the process of somite formation. Somites are paired blocks that produce layered periodical patterns in the developing embryos of animals. Somites appear in the initial stages of morphogenesis, and further, they give rise to different organs, for example, skeletal muscle. The clock and wavefront (CWF) model, first proposed in [25], see also [26], allows us to describe the somite formation as a result of the oscillating expression of genes (which was detected in experiments, see [27]). However, such a model permits us to explain only how periodical gene expression oscillations encode periodical layers. To encode arbitrary patterns we need waves with chaotic dynamics [21]. Chaotic waves also help in practical problems of pattern coding [20].

2. Statement of the Problem

We consider the Cauchy problem for general reaction–diffusion systems:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + F(u), \quad x \in \mathbb{R},\ t \geq 0 \tag{6}$$

with the initial condition

$$u(x,0) = u_0(x). \tag{7}$$

Here, $u = (u_1, \ldots, u_m)$, $F = (F_1, \ldots, F_m)$, and D is a diagonal matrix with positive diagonal elements d_i, $i = 1, \ldots, m$. The function $F(u)$ has the form

$$F(u) = f(u) + \lambda g(u),$$

where $f = (f_1, \ldots, f_m)$, $g = (g_1, \ldots, g_m)$, λ is a small positive parameter, and $f(u)$ satisfies the following conditions:

$$f(u_+) = f(u_-) = 0$$

for some constant vectors u_+ and u_-, $u_- < u_+$ (the inequality is understood component-wise),

$$\frac{\partial f_i(u)}{\partial u_j} \geq 0, \quad i, j = 1, \ldots, m,\ i \neq j,\ u \in B_\kappa, \tag{8}$$

and $f(u) \in C^2(B_\kappa)$. Here, B_κ denotes the set of $u \in R^m$ satisfying the inequality $u_- - \kappa \leq u \leq u_+ + \kappa$, where κ is a small positive number. The main case, where all conditions to f are fulfilled, is given by the relations

$$f_i(u) = u_i - u_i^3, \quad d_i = 1/2. \tag{9}$$

Here, $u_\pm = \pm 1$. Below, we consider this case in order to simplify the statement, and moreover, due to the basic role of the Ginzburg–Landau model in physics.

If $\lambda = 0$ and if we suppose for simplicity that $u_0(\pm\infty) = u_\pm$, then the large-time behaviour of solutions of the Cauchy problem (6) and (7) is described by travelling-wave solutions. We recall that a travelling wave is a solution of the form $u(x,t) = w(x - ct)$. Here, c is an unknown constant, the wave velocity, and the function $w(x)$ is a solution of the problem

$$Dw'' + cw' + f(w) = 0, \quad w(\pm\infty) = u_\pm. \tag{10}$$

In the case (9), this problem is particularly easy: $w(x - q) = \tanh(x - q)$, where q is a constant and $c = 0$, i.e., in this case we are dealing with standing waves. To simplify the subsequent statement, we restrict ourselves by the case (9). The general case of a weakly perturbed monotone system satisfying (8) can be considered in a similar way. Then, we define the non-perturbed kink solution by

$$u_{kink} = W(x,q) = \big(w(x - q_1), \ldots, w(x - q_n)\big), \tag{11}$$

where $q = (q_1, \ldots, q_n)$ is a vector determining the kink positions: q_i defines the position of the kink for the i-th component.

3. Generalized Travelling Waves (GWTs), Universal Dynamical Approximation, and Function Spaces

3.1. GWT

GWTs can be defined as more general solutions

$$u(x,t) = v(x, q_1(t), \ldots, q_m(t)), \tag{12}$$

where the function $q_i(t)$ satisfies the system of ordinary differential equations

$$\frac{dq_i}{dt} = \lambda \Phi_i(q, \lambda),\ i = 1, \ldots, m, \tag{13}$$

where $\Phi(q, \lambda)$ depends on the perturbation g. The existence of such solutions is proved in [15]. Due to the translational invariance of system (6), the right-hand side Φ_i is a function of the difference $q_i - q_l$. We can, thus, reduce (13) to a shorted system

$$\frac{dy_i}{dt} = \lambda \tilde{\Phi}_i(y, \lambda),\ i = 1, \ldots, n, \tag{14}$$

where $n = m - 1$ and $y_i = q_i - q_m$.

Further, we apply the idea of universal dynamical approximation (UDA) (see Appendix A). The right-hand side $\tilde{\Phi}$ in (14) depends on g, it is a linear functional of g. By adjusting the perturbation g, we can approximate any prescribed smooth vector field $Q(y)$ by Φ with an arbitrarily small accuracy $\epsilon > 0$ (in a compact domain which contains an absorbing set of the system $dq/dt = Q(q)$).

This fact, and fundamental results of the theory of dynamical systems (see Appendix A), allows us to prove that there can exist periodic (for $n \geq 3$) and even chaotic (for $n \geq 4$) solutions enjoying special properties. They can describe a collision of wave fronts leading to chaos.

3.2. Function Space and Invariant Manifold

To formulate the results, first let us introduce useful function spaces. Let $E = C(R)$ be the Banach space of bounded continuous functions and $C^2(R)$ the space of functions the first and second derivatives of which belong to $C(R)$. The operator $Au = Du''$, with the domain $D(A) = C^2(R)$, is sectorial in $C(R)$ [28]. (Here, $'$ denotes the derivative with respect to x.) Hence, we can introduce the space $E^\alpha = D(A_1^\alpha)$ with the norm

$$\|u\|_\alpha = \|A_1^\alpha u\|,$$

where $\|\cdot\|$ is the uniform norm, and $\alpha \geq 0$, $A_1 = A - aI$, $a > 0$, I is the identity operator (see [29]).

It is shown [15] that under certain conditions system (6) has an invariant locally attracting manifold M_λ for all sufficiently small $\lambda > 0$. This manifold is a C^1-graph $\tilde{v} = V(q, \lambda)$ in E^α, where $1/2 < \alpha < 1$.

The dynamics of system (6) reduced to M_λ is defined by the system of ordinary differential equations

$$q'(t) = \lambda \Phi(q, \lambda), \tag{15}$$

where $\Phi(q, \lambda)$ is continuous together with its first derivative with respect to q. This function is a sum of the main term $\Phi^{(0)}$ and a perturbation $\Phi^{(1)}$:

$$\Phi(q, \lambda) = \Phi^{(0)}(q) + \Phi^{(1)}(q, \lambda), \tag{16}$$

$$\Phi^{(0)}(q,\lambda) = -\int_{-\infty}^{\infty} g(W(z,q))\ \tilde{U}(z)dz, \tag{17}$$

where $W(z,q)$ is defined by (11),

$$|\Phi^{(1)}(q,\lambda)|,\ |\Phi^{(1)}{}_q(q,\lambda)| < C\lambda, \tag{18}$$

where

$$\tilde{U}(z) = \frac{\sqrt{3}}{2}\cosh^{-2}(z). \tag{19}$$

The system of equations (15) describes a slow motion of the kink system. These equations have a transparent energetic interpretation. Equation (15) for kink coordinates q_i show an energetic balance: the energy dissipation per unit time equals the energy change per unit time due to the kink interaction (see Appendix B).

4. Main Result

The main new result is given by the following theorem.

Theorem 1. *For $n > 3$ there is a smooth function g such that for sufficiently small $\lambda > 0$ systems (15) and (16) have solutions $q(t)$ enjoying the following properties:*

*(**A**) for $0 < t < T$, where $T = o(\lambda^{-1})$, one has*

$$q_i(t) = q_i(0) - \lambda\bar{c}_i t + O(\lambda^2), \tag{20}$$

where $\bar{c}_i$ is a constant which is positive for $i = 1$ and negative for $i = 2,\dots,n$;

*(**B**) for $t >> T$ the dynamics (15) of q_i is defined by chaotic hyperbolic dynamics.*

Comments:

(i) On hyperbolic chaotic dynamics, see [30]. Among systems, which we can find in real applications, the Lorenz system has a dynamical behaviour close to hyperbolic. By adjusting g we can change the chaotic dynamics of q.

(ii) The physical interpretation of this theorem is transparent. First, the fronts (kinks) move independently and, therefore, with almost constant velocities. When the kinks get close to each other they start interacting. This interaction can lead to chaos or periodic oscillations (if the perturbation g is adjusted in an appropriate way) (see Figure 2).

5. Proof

Outline of the proof

Our plan is as follows. First, we prove the existence and boundedness of the solutions; after this, we introduce new coordinates (q,v) in the phase space. The vector q defines the kink coordinates, whereas v is a kink form correction. Using these coordinates, we obtain the existence of a locally invariant n-dimensional manifold. Then, we can describe the dynamics on this manifold. The proof of (**B**) uses some new ideas.

5.1. A Priori Estimates, Global Existence, and Uniqueness

We assume that the function $g(u)$ is smooth, and f is defined by (9).

Lemma 1. *For sufficiently small $\lambda > 0$, there exists a constant vector $b = (b_1,\dots,b_n)$ such that the solution $u(x,t)$ of the Cauchy problem (6) and (7) satisfies the inequality*

$$u_+ - b \le u(x,t) \le u_- + b \tag{21}$$

for all $x \in R$ and $t \ge 0$ if

$$u_+ - b \le u_0(x) \le u_- + b,\quad x \in R. \tag{22}$$

Proof. The proof is standard; see [15]. □

We note that the global existence and uniqueness of the classical solutions of (6) and (7) is well known (see, for example, [3,5]).

A priori estimate (21) implies that for sufficiently small $\lambda > 0$ Equations (6) and (7) generate a semigroup S^t if we restrict ourselves by initial data satisfying (22). If the initial condition u_0 belongs to E^δ for some $\delta > 0$ and satisfies (22), then for any $t > 0$, the solution $S^t u_0$ belongs to E^α for any $0 < \alpha < 1$ and satisfies (21). We denote by $\langle , \rangle$ the inner product in $L_2^m(R)$ and in $L_2(R)$.

5.2. Invariant Manifold

In this subsection, we define an invariant locally attracting manifold M_λ describing the large-time behaviour of the solutions of Equations (6) and (7). If $\lambda = 0$, then this manifold is defined by the relation

$$M_0 = \{u : u = w(x - x^0)\},$$

where $w(x)$ is given by

$$w = (w_1, \dots, w_n)^{tr}, \quad w_i = \tanh(x - x_i^0).$$

The shift x^0 can be considered as a coordinate on this manifold. The global semiflow S^t reduced to M_0 can be described by the equation $dx^0/dt = 0$. It is shown that for small $\lambda \neq 0$ the invariant manifold M_λ still exists and is close to M_0 [15]. We outline it following [15].

5.3. Coordinates in the Neighbourhood of M_0

Denote W_δ^α the neighbourhood of M_0 in the space E^α:

$$W_\delta^\alpha = \{u \in E^\alpha : \inf_{x_0} \|u(z) - w(z - x_0)\|_\alpha < \delta\}. \tag{23}$$

In the case $\alpha = 0$, we use the notation W_δ.

We study solutions of (6) with the initial conditions u_0 from W_δ^α, $\alpha > 0$. Let us introduce new variables (q, v) as follows. For each $u \in W_\delta^\alpha$ we put

$$v(z - q) = u(z) - w(z - q) \in E, \tag{24}$$

where a real number q should satisfy the following equation

$$\rho(q, u) \equiv \langle u(\cdot) - w(\cdot - q), \tilde{U}(\cdot - q)\rangle \equiv \int_{-\infty}^{\infty} (u(z) - w(z - q))\tilde{U}(z - q)dz = 0. \tag{25}$$

Here, $\tilde{U}$ is defined by (19).

Below, we denote by C all positive constants independent of u and λ.

5.4. Change of Variables

Consider the solution $u(x, t)$ of the Cauchy problem (6) and (7). Suppose that $u(z, t) \in W_\delta^\alpha$ for $0 \leq t \leq T$ for some $T > 0$. For each t fixed, we define $q(t)$ and $v(\xi, t)$ by the following relations:

$$\rho(q, u(\cdot, t)) = 0, \quad v(\xi, t) = u(\xi + q(t), t) - w(\xi). \tag{26}$$

The function $q(t)$ determines the shift of the unperturbed wave and v is a perturbation of the wave. Equations (6) and (7) reduce to system (15) in a small neighbourhood of locally attracting invariant manifold [15].

5.5. Concluding Steps

The idea is illustrated by Figures 1 and 2. We suppose that the nonlinearity f has the form (9). Consider a system of ordinary differential equations

$$\frac{dy}{dt} = Q(y), \quad y \in \mathbb{R}^n \tag{27}$$

where $Q(y) \in C^2(\mathbb{R}^n)$. Suppose that B is a bounded domain in $\mathbb{R}^n$ with a smooth boundary ∂B such that

$$y \cdot Q(y) = \sum_{i=1}^{n} y_i Q_i < -\delta_1, \quad \delta_1 > 0, \quad \text{if } y \in \partial B \tag{28}$$

i.e., the corresponding vector field on the boundary ∂B fits inside B. This means that the set B is absorbing. We suppose that dynamics (27) has hyperbolic invariant set Γ, which lies inside B: $\Gamma \subset B$.

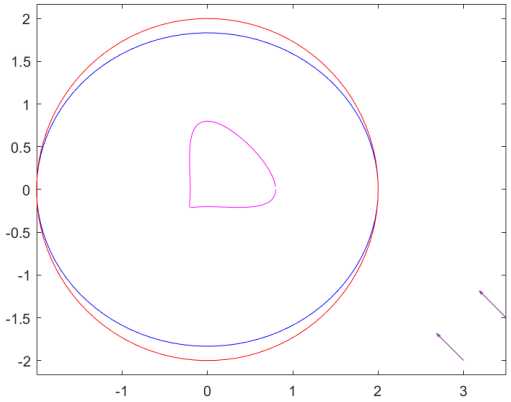

Figure 1. This image shows the main idea of the proof. Let y be the mutual distances between kinks (see proof). We have the two domains in the y-space $\mathbb{R}^n$ (in this image $n = 2$), B_δ and B', and a structurally stable attractor $\mathcal{A}$. There are embeddings $\mathcal{A} \subset B' \subset B_\delta$. These domains are shown as ellipses. The attractor $\mathcal{A}$, which is a limit cycle, is shown by a closed curve. The vector field $Y(y)$ is equal to a constant vector field $\bar{c}$ outside of B_δ (it is shown by arrows). In the transient domain $B_\delta - B'$ we have a smooth homotopy between the constant field $\bar{c}$ and Q. We choose the field $\bar{c}$ as follows: (a) it should be directed toward the interior of B_δ at a part ∂E of the boundary ∂B_δ; (b) some components of the vector $\bar{c}$ must be positive and other ones are negative. Condition (a) implies that the y-trajectories enter for absorbing set B'. Therefore, for large times t these trajectories are defined by the attractor $\mathcal{A}$. Condition (b) entails that the y-dynamics describes a collision of travelling fronts (see the next image).

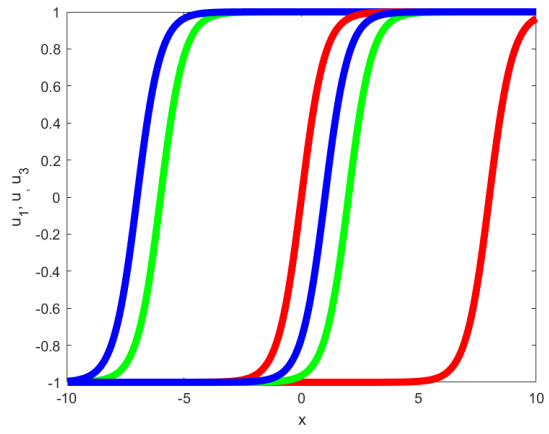

Figure 2. This image shows the time evolution of travelling fronts (kinks) under condition (b) of the previous image. At the initial moment $t = 0$ the kinks are far from each other. The kink velocities and their initial coordinates can be chosen so that when the kink coordinates $q(t)$ approach the boundary of the domain B_δ, they end up on the boundary set ∂E, where the trajectories of the semiflow S_Y^t enters for B_δ. Beginning with this moment, the kinks interact and form a connected state. Their coordinates can evolve in time in a periodical (for $m > 2$) or chaotic manner (for $m > 3$).

As an example, we can consider the Lorentz system, which has the form

$$\frac{dy_1}{dt} = \sigma(y_2 - y_1), \quad \frac{dy_2}{dt} = ry_1 - y_1y_3 - y_2, \quad \frac{dy_3}{dt} = y_1y_2 - by_3.$$

Depending on the positive parameters b, r, and σ, the solution of these equations can have convergent, periodic, or chaotic behaviour. Then, the absorbing set B is defined by

$$B = \{y : y \in \mathbb{R}^3, \quad ry_1^2 + y_2^2 = b(y_3 - r)^2 \leq br^2\}.$$

Note that the dynamics of system (27) on the hyperbolic set Γ is structurally stable due to the theorem on the persistence of hyperbolic sets (see [31–33] and Appendix A). This implies that there is a small constant $\varepsilon > 0$ such that if we perturb the field Q by a perturbation $\tilde{Q}$, which is ε small in C^1 norm on the absorbing set, then the perturbed system (27) defined by the vector field $Q + \tilde{Q}$ also has a hyperbolic invariant set Γ', which is topologically equivalent to Γ, close to Γ and the dynamics of the perturbed system restricted to Γ' is orbitally topologically equivalent to the dynamics (27) restricted to Γ.

Our first step is to compress the domain B. We define a family of vector fields $Q_\delta = Q(\delta^{-1}y)$, where $\delta \in (0, 1)$ is a positive constant. Note that $|Q_\delta|_{C^1(B)} < c\delta^{-1}$. System (27) becomes

$$\frac{dy}{dt} = \delta Q(\delta^{-1}y), \quad y \in \mathbb{R}^n \tag{29}$$

It is clear that this system is equivalent to (27) and it has an absorbing set B_δ such that $diam(B_\delta) = O(\delta)$. We can take such a $\delta \in (0, 1)$ that the B_δ is contained in the ball in $\mathbb{R}^n$ of radius $1/2$ centred at 0. This absorbing set B_δ contains the attractor $\mathcal{A}$ of the system (29). Then, there is an open domain B' with a smooth boundary $\partial B'$ such that

$$\mathcal{A} \subset B' \subset B_\delta.$$

Moreover, one can suppose that B' is sufficiently close to B_δ:

$$\inf_{\{y \in \partial B_\delta,\ \tilde{y} \in \partial B'\}} |y - \tilde{y}| > \delta_0, \tag{30}$$

$$\sup_{\{y \in \partial B_\delta,\ \tilde{y} \in \partial B'\}} |y - \tilde{y}| < 2\delta_0, \tag{31}$$

where ∂X denotes the boundary of a set X and δ_0 is a small positive number such that $\delta_0 << \delta$. If $\delta_0 > 0$ is small enough, then B' is also an absorbing set such that the field Q is directed toward to the interior of B' at ∂B_δ.

Let us set $m = n + 1$ and let us define g_i by

$$g_i(u_1, \ldots, u_m) = (2\pi)^{-1/2} p^{-1} \exp(-u_i^2/2p^2) P_i(u_1, \ldots, u_m), \tag{32}$$

where $p > 0$ is a small parameter such that $p << \varepsilon$ (where ε is the constant of persistence introduced above and depending on the field Q only) and P_i are smooth functions of u, which will be adjusted later. We note that g_i is well localized at $u_i = 0$. The value $u_i = 0$ corresponds to $x = q_i$. We substitute g_i from (32) into the right-hand side of (17) and by the standard Laplace method we obtain an asymptotic estimate of the integral on the right-hand side of (17) that gives

$$\Phi_i^{(0)}(q) = \bar{\Phi}_i(q) + p\phi^0(q),$$

where $\phi^0(q)$ is a small smooth correction bounded in $C^2(\mathbb{R}^n)$ norm and

$$\bar{\Phi}_i = P_i\big(\tanh(q_i - q_1), \tanh(q_i - q_2), \ldots, \tanh(q_i - q_m)\big).$$

To simplify computations, we set

$$P_m(u) = \bar{C}_m = const.$$

We introduce new variables y_i by $y_i = q_i - q_m$, $i = 1, \ldots, n$. These variables are convenient to take into account the translation invariance of our problem. Then, $q_i - q_l = y_i - y_l$, where $i, l \in \{1, \ldots, n\}$. Note that the variables (y, q_m) have a clear meaning: the quantity q_m determines the speed of movement of the kink system as a whole, and the quantity y determines the mutual distances between the kinks.

In these new variables, the system of differential equations for q reduces to the following system for y:

$$\frac{dy_i}{dt} = Y_i(y) + \tilde{Y}_i(y), \tag{33}$$

where $i = 1, \ldots, n$ and

$$Y_i(y) = P_i(\tanh(y_i - y_1), \tanh(y_i - y_2), \ldots, \tanh(y_i - y_n), \tanh(y_i)) - \bar{C}_m,$$

$$|\tilde{Y}_i|_{C^1(\mathbb{R}^m)} < c_1 p,$$

where c_1 is a positive constant uniform in p and λ. Let $r(y)$ be the distance between a point y and the set B'. This distance r equals the distance between y and the boundary $\partial B'$ when y lies outside of B', and $r = 0$ if y lies inside B'. We define Y as

$$Y_i = Q_i(y)\chi_{\delta_0}(r) + \bar{c}_i(1 - \chi_{\delta_0}(r))), \tag{34}$$

where $\chi_{\delta_0}(r)$ is a C^2-smooth monotone increasing function defined on $[0, \infty)$ such that

$$\chi_{\delta_0}(r) \equiv 1, \quad 0 < r < \delta_0/2,$$

$$\chi_{\delta_0}(r) \equiv 0, \quad r > \delta_0.$$

Relation (34) means that outside a neighbourhood of B the field Y equals the constant vector $\bar{c} = (\bar{c}_1, \ldots, \bar{c}_n)$, whereas inside B this field equals Q. It is clear that one can choose appropriate functions $P_i(y)$ such that the relation (34) holds. Then the theorem on the persistence of hyperbolic sets [31,32] implies that with g defined by (16), sufficiently small $p, \lambda > 0$ and appropriate δ, δ_0 the y-dynamics defined by the system $dy/dt = Y(y)$ generates a hyperbolic chaotic dynamics if a hyperbolic chaotic dynamics exists for system (27) (see Appendix A).

The proof is complete.

5.6. Effects of Dependence on Initial Data

The front collisions exhibit interesting phenomena of dependence on initial data (initial kink coordinates). Consider Figure 1. We see that depending on the initial data $y(0)$ the y-trajectories can either enter an absorbing set, or pass by. In the latter case, chaos is absent and we have usual travelling waves. The kink speed oscillations are of the order $O(\lambda^2)$. Figure 3 shows the case where all the trajectories enter the absorbing set; therefore, we observe the complicated large-time behaviour of interacting fronts. However, there appears an additional interesting effect: the speeds of the travelling fronts depend on the initial data. This dependence is smooth.

Bistability effects are illustrated by Figure 4. The prescribed dynamics has two local attractors, each attractor has its own area-of-attraction basin. The y-trajectories are defined by a constant vector field, these trajectories enter different attractors depending on their initial data. For some initial data, chaotic or periodical large-time behaviour does not occur.

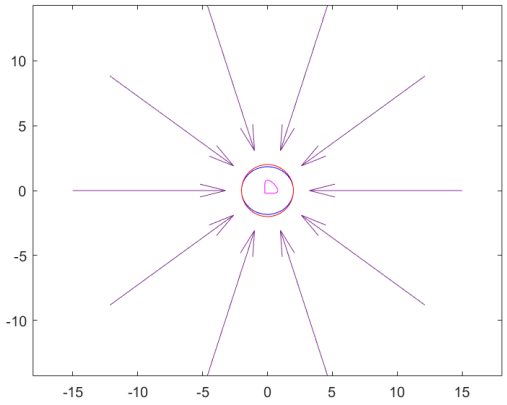

Figure 3. This image shows the case where the front collision leads to periodical large-time behaviour of interacting fronts for all initial data. In this case the fronts have different speeds for different initial data.

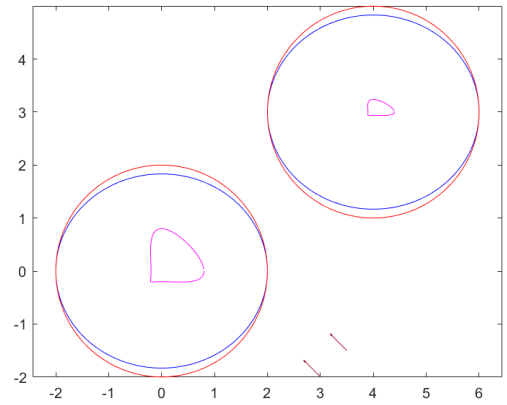

Figure 4. This image shows the case where we have a bistable situation. The prescribed dynamics has two local attractors, each attractor has its own area-of-attraction basin. The y-trajectories, defined by a constant vector field and shown by arrows, enter different attractors depending on the initial data. Some trajectories pass by the attractors.

6. Concluding Remarks

What can happen when chemical waves meet? This is a hard problem, with theoretical results obtained for waves described by reaction–diffusion equations and monotone reaction–diffusion systems. For the most important case of non-monotone systems this problem has been studied in a few works using numerical methods (for example, [34]).

In this paper, based on some previously obtained results, we propose the first model, which allows us to investigate this problem on chemical wave collisions using analytical methods. We show that this reaction–diffusion model exhibits a rich variety of non-trivial phenomena.

The results presented show that for the case of four components the collision of travelling fronts can generate chaotic waves and for the case of three components this collision can generate time-periodic waves. There arise interesting effects of dependency on the initial data: depending on the initial positions we obtain either chaos, periodical dynamics, or convergent dynamics, when the result of the wave meeting is a new travelling front.

These phenomena have a transparent physical interpretation. The wave fronts come closer and form a bound state where the waves interact by exchanging energy. For each reagent, dissipation, associated with wave motion, is equal to an energy transferred from other reagents. Such effects are possible in open systems only, and some reagents should be activators, whereas other are inhibitors.

To conclude let us note the following. Assume we would like to have a very complicated wave motion, say, with an attractor of fractal dimension 100. Then, the method of this paper needs a system with >100 reagents. There arises a natural question: is it possible

to obtain such a complicated behaviour (have an attractor of dimension 100) with only two reagents? It is possible for reaction–diffusion systems in multidimensional domains [35]. Whether it is true or not for the one-dimensional case is as yet unknown.

Finally, we conclude that the possibility of the emergence of complex dynamic regimes as a result of the interaction of waves is shown by rigorous methods. We think that complex coherent waves of gene expression found in Drosophila morphogenesis [36] (see, in particular, Figure 2 from this paper) and neurodynamics [37] cannot be explained by the usual approach based on travelling fronts of constant form and velocity. We believe, therefore, that the generalized travelling front concept could be useful in the future to handle data on gene expression where we are dealing with many genes. In [36], the gene expression was measured for a hundred genes in the time course of the Drosophila embryo's development. It was shown that there exist six temporal waves of coherent gene expression during this Drosophila morphogenesis. Moreover, it was found that the most powerful gene expression waves correspond to great morphogenetic movements. The time-duration analysis of Drosophila embryogenesis first made in [36] reveals a connection between waves of gene expression and morphogenetic processes. The coherent gene expression means that the genes and the corresponding waves interact. Such spatio-temporal patterns of gene expression corresponding to many interacting gene waves are similar to wave patterns, which can be described using generalized travelling waves. In fact, it is impossible to describe the complex gene patterns existing in real organisms by usual travelling waves. Consider a simple example. Gene expression leads to cell differentiation, and different cells form tissues. To explain, for example, a periodic pattern corresponding to the stripes of a zebra's skin, it is sufficient to have a single morphogen with two expression levels, high and low. Depending on these expression levels, the morphogen can induce black (B) or white (W) cells. By a usual travelling wave one can obtain a periodic sequence of cells, say, BWBW.... However, to encode a non-periodic pattern, say, BWAE BWW EEE..., we need a whole group of genes and their complex expression depending on spatial localization. These cellular patterns can be obtained using generalized travelling fronts; see [21] for more details. We think, therefore, that the generalized travelling front concept can be useful in the future to handle such data on gene expression, in particular, when we are dealing with many genes.

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Appendix A. Universal Dynamical Approximation

Let us recall the concept of the realization of the vector fields for dissipative systems proposed by P. Poláčik in [38]. For definiteness, we consider the case of a system with continuous time (the case of iterations is treated similarly). We consider dynamical systems which enjoy the following properties **A** and **B**:

A *Dynamical systems (defined by vector field F) generate global semiflows $S^t_{\mathcal{P}}$ in an ambient Hilbert or Banach phase space H. These semiflows depend on some parameters $\mathcal{P}$ (which could be elements of another Banach space $\mathcal{B}$). They have global attractors and finite-dimensional locally attracting invariant C^1-manifolds $\mathcal{M}$, at least for some $\mathcal{P}$.*

B *The dynamics of $S^t_{\mathcal{P}}$ reduced to the invariant manifolds can be almost completely tuned by variations of the parameter $\mathcal{P}$.*

This can be described as follows. Assume that the differential system

$$\frac{dq}{dt} = Q(q), \quad Q \in C^1(B_R^n) \tag{A1}$$

defines a global semiflow in a ball $B_R^n \subset \mathbf{R}^n$ of radius $R > 0$ centred at 0.

For any prescribed dynamics (A1) and any $\epsilon > 0$, one can choose suitable parameters $\mathcal{P} = \mathcal{P}(n, F, \epsilon)$ such that

1. the semiflow $S_{\mathcal{P}}^t$ has a C^1-smooth locally attracting invariant manifold $\mathcal{M}_{\mathcal{P}}$ diffeomorphic to B^n;
2. the reduced dynamics $S_{\mathcal{P}}^t|_{\mathcal{M}_{\mathcal{P}}}$ is defined by equations

$$\frac{dq}{dt} = \tilde{Q}(q, \mathcal{P}), \quad \tilde{Q} \in C^1(B^n), \tag{A2}$$

where

$$|Q - \tilde{Q}|_{C^1(B^n)} < \epsilon. \tag{A3}$$

According to the terminology introduced by [38] we say that our family of semiflows ϵ-realizes the vector field Q if the estimate (A3) holds. The properties **A** and **B** mean that our class system realizes all finite dimensional vector fields, with an arbitrarily high accuracy. In other words, one can say that by tuning $\mathcal{P}$, the reduced dynamics on the invariant manifold can be specified with an arbitrarily small error. Therefore, roughly speaking, all robust dynamics (stable under small perturbations) can be generated by systems which satisfy the above formulated properties. Such systems are denoted as *UDA systems* (systems having the property of universal dynamical approximation). In order to show that the UDA concept also covers the case of chaotic dynamics, let us recall some facts about chaos and hyperbolic sets. Let us consider systems of differential equations defined by (A2) which satisfy the following conditions:

Condition on the structural stability of prescribed dynamics (SSPD). *System* (A2) *generates a global semiflow* S^t, $t > 0$, *defined on the n-dimensional closed ball* $B^n \subset \mathbb{R}^n$ *and having structurally stable (for example, hyperbolic) local attractors* $\mathcal{A}_l$, $l = 1, \ldots, k$.

Comment. Recall that structural stability is a fundamental property of dynamics, which means that the topological structure of the trajectories of the system (A2) on $\mathcal{A}_l$ are unaffected by C^1-small perturbations of the vector field Q. In particular, under small perturbations hyperbolic rest points remain so and only slightly shift, they cannot be transformed into cycles, and vice versa, hyperbolic cycles cannot become points.

These attractors can have a complex form, since structurally stable dynamics may be *chaotic*. If a hyperbolic invariant set Γ is attracting and this set is not a rest point or a limit cycle, we say that Γ is a chaotic (strange) attractor [31]. Hyperbolic sets have a fundamental property of hyperbolic sets, so-called *persistence*. Informally speaking, this means that the hyperbolic sets are stable (robust) with respect to small sufficiently smooth perturbations (see [31] for details).

Appendix B. Energetic Interpretation of Equations for Kink Coordinates

The system of equations (15) describes a slow motion of a kink system. These equations have a transparent energetic interpretation. Let us multiply the equation for u_i by $\frac{\partial u_i}{\partial t}$ and integrate over all x. Then, we have

$$K_i = -dE_i/dt + \lambda R_i, \tag{A4}$$

where

$$K_i = \int_{-\infty}^{\infty} (\frac{\partial u_i}{\partial t})^2 dx,$$

$$E_i = \frac{1}{4} \int_{-\infty}^{\infty} \Big((\frac{\partial u_i}{\partial x})^2 + (1 - u_i^2)^2 \Big) dx$$

and

$$R_i = \int_{-\infty}^{\infty} g_i(u,x)\frac{\partial u_i}{\partial t}dx.$$

The relation (A4) shows an energetic balance. The term K_i is always positive and defines the energy dissipation, the term E_i is a non-perturbed kink energy and the term R_i shows the change in energy due to the perturbation g_i. If we substitute into K_i the unperturbed kink solution $u_i(x - q_i(t))$ (removing the terms that describe the deformation of the kink form), we obtain that

$$K_i \approx (\frac{dq_i}{dt})^2 \int_{-\infty}^{\infty} \tilde{\mathcal{U}}^2 dx. \tag{A5}$$

Here, and below, the symbol $\approx$ means that we take into account only the main terms as $\lambda \to 0$, for example, $\lambda + 2\lambda^2 \approx \lambda$. The same substitution gives $E_i \approx 0$ that is a consequence of translation invariance, and

$$R_i \approx \frac{dq_i}{dt} \int_{-\infty}^{\infty} g_i(u_{kink}(x,q),x)\tilde{\mathcal{U}}dx. \tag{A6}$$

We substitute these asymptotics for K_i, E_i, and R_i into (A4) and see that

$$(\frac{dq_i}{dt})^2 \approx Q_i(q)\frac{dq_i}{dt} \tag{A7}$$

is equivalent to (15). We obtain, thus, that the main motion, Equation (15), for kinks represents an energetic balance: the energy dissipation per unit time K_i equals the energy change per unit time R_i due to the kink interaction.

A rigorous derivation of Equation (15) for kink coordinates can be found in [15].

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