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The Hamiltonian formalism in reaction-diffusion systems

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Abstract.

It is well known that the Hamiltonian formalism plays an central role in classical mechanics. In this survey, we show that the Hamiltonian formalism is useful for studying pattern formation problems in reaction-diffusion systems. Although they are not derived from the Newton principle (the motion law), the notion of gradient/skew-gradient structure enables us to use the Hamiltonian formalism for their study. This structure was originally introduced by [14], and formulated in more abstract fashion by [6]. We explain usefulness of the gradient/skew-gradient structure through the linear stability analysis of standing pulse solutions and spatially periodic patterns in reaction-diffusion systems of activator-inhibitor type.

keywords: gradient/skew-gradient structure, Hamiltonian formalism, pattern formation, reaction-diffusion systems

§1. Introduction

There are many interesting macro scopic spatio-temporal patterns in dissipative systems such as chemical reaction and biological morphogenesis, which are maintained by balance between supply and consumption of energy and substances. The dynamics of such patterns are often described by a system of reaction-diffusion equations [10, 11], which is a phenomenological model derived from careful observations based on real and/or numerical experiments. Therefore it is not always easy to perform theoretical analysis of a proposed reaction-diffusion system even if it is a good model which describes the dynamics of patterns.

On the other hand, various interesting spatio-temporal patterns have attracted much attention in dynamics of a fluid and a motion of rigid

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bodies. The dynamics of these patterns are described by the equation of motion derived from the Newton principle. The theory of classical mechanics established by Euler, Lagrange, Hamilton and Jacobi provides an useful framework for studying the equation of motion. It plays a central role in hydrodynamics and the theory of rigid-body dynamics [1, 7].

The aim of this survey is to explain that the Hamiltonian formalism in classical mechanics is useful for studying pattern formation problems in reaction-diffusion systems. As is mentioned above, since they are phenomenological models not derived from the Newton principle, the Hamiltonian formalism is not always applicable to analysis of them. However, the gradient/skew-gradient structure introduced in the next section enables us to apply the Hamiltonian formalism to the study of reaction-diffusion systems. This structure was originally introduced by [14], and formulated in more abstract fashion by [6]. The organization of this survey is as follows: In the next section, we introduce the gradient/skew-gradient structure following [6]. In section 3, according to [14], we review the linear stability analysis of standing pulse solutions in reaction-diffusion systems. The gradient/skew-gradient structure enables us to compute the eigenfunctions of the adjoint operator of the linearized eigenvalue problem at a standing pulse. In section 4, we explain the linear stability analysis of spatially periodic steady states in reaction-diffusion systems with the gradient/skew-gradient structure [6]. It is a typical example to understand usefulness of the Hamiltonian formalism for studying reaction-diffusion systems. Section 5 is devoted to a brief summary of this survey.

§2. Reaction-diffusion systems with gradient/skew-gradient structure

As was mentioned in the previous section, a reaction-diffusion system gives a phenomenological model for studying dynamics of dissipative systems. For example, the Ginzburg-Landau equation

$$(2.1) \qquad \left\{ \begin{array}{lcl} u_t & = & u_{xx} + u(1 - u^2 - v^2) \\ v_t & = & v_{xx} + v(1 - u^2 - v^2) \end{array} \right.$$

is a very famous reaction-diffusion system in the study of phase transition phenomena. We can easily (formally) find that (2.1) has gradient structure, i.e., an energy equation

$$\frac{d}{dt}\tilde{E}[u(x,t), v(x,t)] = -\int (u_t^2 + v_t^2)\, dx$$

holds, where

$$\tilde{E}[u,v] = \int \{ \frac{1}{2}(u_x^2 + v_x^2) + \frac{1}{4}(1 - u^2 - v^2)^2 \} \, dx.$$

It is well known [11] that many interesting results concerning (2.1) have been obtained by mathematical analysis based on the gradient structure of (2.1). The notion of gradient/skew-gradient structure introduced in this survey is an extension of the gradient structure explained in the above example.

Let us consider an n-component reaction-diffusion system

$$Tu_t = D \triangle u + f(u), \quad u = (u_1, u_2, \cdots, u_n), \quad x \in \mathbf{R}^N. \tag{2.2}$$

According to [6], the reaction-diffusion system is said to have gradient/skew-gradient structure when (2.2) satisfies the following assumptions:

(A1) T is a non-degenerate positive diagonal matrix.
(A2) D is a regular matrix satisfying $D^T Q = QD$, where Q is a symmetric matrix with $Q^2 = I_n$.
(A3) $f(u) = Q\nabla_u F(u)$, where $F = F(u) : \mathbf{R}^n \to \mathbf{R}$ is a smooth function.

Under the above assumptions, we immediately see that QD is a symmetric matrix, and that the Jacobi matrix of f denoted by f_u satisfies

$$f_u(u)^T Q = Q f_u(u). \tag{2.3}$$

Moreover, (2.2) has a (skew) energy functional defined by

$$\tilde{E}[u] = \int \left\{ \frac{1}{2} \langle\langle D\nabla u, Q\nabla u \rangle\rangle - F(u) \right\} dx,$$

where

$$\langle\langle D\nabla u, Q\nabla u \rangle\rangle := \sum_{i,j} d_{ij} \nabla u_j \cdot q_{ij} \nabla u_j.$$

In fact, we can easily (formally) check that the (skew) energy equation

$$\frac{d}{dt} \tilde{E}[u(x,t)] = - \int \langle u_t, QTu_t \rangle \, dx$$

holds, where $\langle \; , \; \rangle$ denotes the usual inner product defined on $\mathbf{R}^n$. (2.2) is said to have gradient structure when QT is nonnegative symmetric, and skew-gradient structure otherwise.

An example of reaction-diffusion system with gradient structure is given by the Ginzburg-Landau equation (2.1). As for an example of skew-gradient reaction-diffusion system, we give a reaction-diffusion system of activator-inhibitor type as follows:

$$\tau_1 u_t = d_1 \triangle u + \alpha u - u^3 - v, \quad \tau_2 v_t = d_2 \triangle v + u - \beta v. \tag{2.4}$$

In fact, we can easily verify that (2.4) satisfies the assumptions (A1)-(A3) because it is rewritten in the form of (2.2) with

$$T = \begin{pmatrix} \tau_1 & 0 \\ 0 & \tau_2 \end{pmatrix}, \quad D = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}, \quad Q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$F = F(u, v) = \frac{1}{2}\alpha u^2 - \frac{1}{4}u^4 - uv + \frac{1}{2}\beta v^2.$$

For other examples, see [6].

In what follows, we consider (2.2) in one-dimensional case $N = 1$, that is,

$$Tu_t = Du_{xx} + f(u), \quad u = (u_1, u_2, \cdots, u_n), \quad x \in \mathbf{R}. \tag{2.5}$$

Then, the equation for stationary solutions of (2.5)

$$Du_{xx} + f(u) = 0 \tag{2.6}$$

admits structure of the Hamiltonian dynamical systems. Indeed, setting $u_x = v$, (2.6) can be rewritten as a first order system

$$u_x = v, \quad Dv_x = -f(u),$$

which leads to

$$QDu_x = QDv, \quad QDv_x = -Qf(u).$$

As a consequence, it turns out that (2.6) is rewritten in the canonical form

$$KZ_x = -\nabla_Z H(Z), \tag{2.7}$$

where $Z = (u, u_x)^T$ and

$$K = \begin{pmatrix} 0 & QD \\ -QD & 0 \end{pmatrix} \tag{2.8}$$

is a skew-symmetric matrix because QD is symmetric, and $H(Z)$ is a first integral (Hamiltonian) given by

$$H(Z) = H(u, u_x) := \frac{1}{2}\langle Du_x, Qu_x\rangle + F(u). \tag{2.9}$$

Thus we expect that the theory of Hamiltonian dynamical systems can be applied for studying various properties of stationary solutions of (2.5). In section 4, we show that the canonical form (2.7) is useful in the stability analysis of spatially periodic stationary solutions of (2.5).

§3. Stability analysis of standing pulse solutions

In this section, according to [14], we review a strategy of the linearized stability analysis of a standing pulse solution of (2.5) with the skew-gradient structure. For more details, the reader should consult [14]. Let us consider

$$D\phi_{xx} + f(\phi) = 0, \qquad \phi(x) = p + O(e^{-C|x|}) \quad \text{as } x \to \pm\infty, \tag{3.1}$$

where C is a positive constant, and $p \in \mathbf{R}^n$ satisfies $f(p) = 0$.

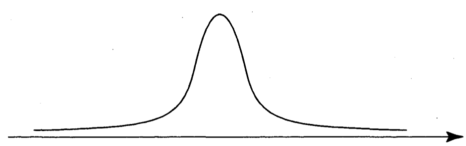

Figure 1 : the shape of a standing pulse

We call ϕ a standing pulse solution of (2.5). Notice that ϕ represents any stationary solution of (2.5), which decays exponentially as $x \to \pm\infty$. A typical example of the shape of ϕ is presented in Figure 1. In order to investigate the stability of ϕ, we are concerned with the linearized eigenvalue problem of (2.5) at ϕ defined by

$$\lambda Tv = Dv_{xx} + f'(\phi)v \tag{3.2}$$

on the space $C^0_{unif}(\mathbf{R})$ of bounded uniformly continuous functions. Setting $Y = (v,\, v_x)^T$, we rewrite (3.2) as a first-order ODE

$$Y_x = A(x)Y + \lambda BY, \tag{3.3}$$

where

$$A(x) = \begin{pmatrix} 0 & I_n \\ -D^{-1}f'(\phi) & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ D^{-1}T & 0 \end{pmatrix}.$$

We can regard (3.3) as a system of linear ODEs with constant coefficients

$$Y_x = AY + \lambda BY, \qquad A = \begin{pmatrix} 0 & I_n \\ -D^{-1}f'(p) & 0 \end{pmatrix} \tag{3.4}$$

as $x \to \pm\infty$.

According to [13], λ is in the essential spectrum of the linear operator associated with the eigenvalue problem (3.2) if

$$\det(A + \lambda B - ik) = 0$$

has a solution $k \in \mathbf{R}$. That is, $A + \lambda B$ has an eigenvalue with zero real part, i.e., $\operatorname{spec}(A + \lambda B) \cap i\mathbf{R} \neq \emptyset$

From now on, we are concerned with the point spectrum of the linear operator associated with the eigenvalue problem (3.2). Namely, we consider $\lambda \in \mathbf{C}$ such that all the eigenvalues of $A + \lambda B$ have nonzero real part, i.e., $\operatorname{spec}(A+\lambda B) \cap i\mathbf{R} = \emptyset$. In this case, (3.4) has m and $2n-m$ linearly independent exponentially decaying solutions as $x \to -\infty$ and $x \to +\infty$, respectively.

Differentiating (3.1) with respect to x, we have

$$D\phi'_{xx} + f'(\phi)\phi' = 0, \qquad \phi'(x) = O(e^{-C|x|}) \quad \text{as } x \to \pm\infty,$$

which implies that (3.3) has m and $2n - m$ linearly independent exponentially decaying solutions $Y_j(x;\lambda)$ $(j = 1, 2, \cdots m)$ and $Y_k(x;\lambda)$ $(k = m, m+1, \cdots 2n)$ with

$$Y_1(x;0) = Y_{2n}(x;0) = \Phi(x), \quad \Phi(x) = \begin{pmatrix} \phi'(x) \\ \phi''(x) \end{pmatrix} \tag{3.5}$$

as $x \to -\infty$ and $x \to +\infty$, repectively. Then, a bounded solution of (3.3) is expressed by

$$Y(x) = c_1 Y_1(x;\lambda) + \cdots + c_m Y_m(x;\lambda) = c_{m+1} Y_{m+1}(x;\lambda) + \cdots + c_{2n} Y_{2n}(x;\lambda)$$

Therefore, $Y_j(x;\lambda)$ $(j = 1, 2, \cdots 2n)$ must be linearly dependent when (3.3) has a non-trivial bounded solution. Namely,

$$E(\lambda) = \det(Y_1(0;\lambda)\ Y_2(0;\lambda)\ \cdots\ Y_{2n}(0;\lambda)) = 0 \tag{3.6}$$

holds if and only if λ is in the point spectrum of the eigenvalue problem (3.2). The function $E(\lambda)$ is called the Evans funtion which plays a crucial role in the stability analysis of the standing pulse ϕ.

We immediately find that $E(0) = 0$ by (3.5). Moreover, it follows from [13, Section 4.2.2] that $E(\lambda) > 0$ for sufficiently large $\lambda > 0$. Hence, if $E'(0) < 0$, then $E(\lambda_0) = 0$ holds for some $\lambda_0 > 0$, so that (3.3) has a non-trivial bounded solution for some $\lambda_0 > 0$. Therefore, the standing pulse ϕ is linearly unstable provided $E'(0) < 0$.

Differentiating (3.6) with respect to λ, and setting $\lambda = 0$, we have

$$\begin{aligned} E'(0) &= \det(\ \partial_\lambda Y_1(0;\lambda)\ Y_2(0;\lambda)\ \cdots\ Y_{2n}(0;\lambda)\ )|_{\lambda=0} \\ &\qquad + \det(\ Y_1(0;\lambda)\ Y_2(0;\lambda)\ \cdots\ \partial_\lambda Y_{2n}(0;\lambda)\ )|_{\lambda=0} \\ &= \det(\ Y_1(0;\lambda)\ \cdots\ Y_{2n-1}(0;\lambda)\ \partial_\lambda(Y_{2n}(0;\lambda) - Y_1(0;\lambda))\ )|_{\lambda=0}, \end{aligned}$$

because $Y_1(0;0) = Y_{2n}(0;0)$ by virtue of (3.5). We can compute the value of this determinant as long as we know the orthogonal projection of $\partial_\lambda(Y_1(0;\lambda) - Y_{2n}(0;\lambda))|_{\lambda=0}$ to $W^\perp$, where $W = \operatorname{span}\{Y_1(0;0),\ Y_2(0;0),\ \cdots,\ Y_{2n-1}(0;0)\}$.

On the other hand, by using $Y^*(x;\lambda)$ a solution of the adjoint system of (3.3) defined by

$$Y^*_x = -A(x)^T Y^* - \lambda B^T Y^*, \tag{3.7}$$

we have

$$\begin{aligned} &\frac{d}{dx}\langle Y_j(x;\lambda),\ Y^*(x;\lambda)\rangle \\ &= \langle\ \frac{d}{dx}Y_j(x;\lambda),\ Y^*(x;\lambda)\rangle + \langle Y_j(x;\lambda),\ \frac{d}{dx}Y^*(x;\lambda)\ \rangle \\ &= \langle\ (A(x)+\lambda B)Y_j(x;\lambda),\ Y^*(x;\lambda)\rangle + \langle Y_j(x;\lambda),\ -(A(x)+\lambda B)^T Y^*(x;\lambda)\ \rangle \\ &= 0, \quad (j = 1, 2, \cdots, 2n). \end{aligned}$$

Hence, it follows from $Y_j(x;\lambda) \to 0$ as $x \to +\infty$ or $x \to -\infty$ that

$$W^\perp = \operatorname{span}\{\Psi^*(0)\}$$

holds, where Ψ^* is defined by a bounded solution of

$$\Psi^*_x = -A(x)^T \Psi^*. \tag{3.8}$$

Differentiating (3.3) and (3.7) with respect to λ, and using (3.5), a direct calculation yields

$$\begin{aligned} &\langle \partial_\lambda(Y_1(0;\lambda) - Y_{2n}(0;\lambda))|_{\lambda=0},\ \Psi^*(0)\rangle \\ &= \int_{-\infty}^0 \langle \frac{d}{dx}\partial_\lambda Y_1(x;0) - A(x)\partial_\lambda Y_1(x;0), \Psi^*(x)\rangle dx \\ &\qquad + \int_0^\infty \langle \frac{d}{dx}\partial_\lambda Y_{2n}(x;0) - A(x)\partial_\lambda Y_{2n}(x;0), \Psi^*(x)\rangle dx \\ &= \int_{-\infty}^\infty \langle B\Phi(x),\ \Psi^*(x)\rangle dx. \end{aligned}$$

Since the orthogonal projection of $\partial_\lambda(Y_1(0;\lambda) - Y_{2n}(0;\lambda))|_{\lambda=0}$ to $W^\perp$ is given by

$$\left\langle \partial_\lambda(Y_1(0;\lambda) - Y_{2n}(0;\lambda))|_{\lambda=0},\ \frac{\Psi^*(0)}{|\Psi^*(0)|} \right\rangle \frac{\Psi^*(0)}{|\Psi^*(0)|},$$

we obtain

(3.9)

$$E'(0) = \int_{-\infty}^{\infty} \langle B\Phi(x),\ \Psi^*(x)\rangle dx \cdot \frac{\det(\ Y_1(0;0)\ \cdots\ Y_{2n-1}(0;0)\ \Psi^*(0))}{\langle \Psi^*(0),\ \Psi^*(0)\rangle},$$

where

$$\int_{-\infty}^{\infty} \langle B\Phi(x),\ \Psi^*(x)\rangle dx \tag{3.10}$$

is called the Melnikov integral. In many practical problems, the stability of standing pulse solutions of (2.5) is determined by the signature of the Melnikov integral (3.10). Notice that (3.9) holds for any general reaction-diffusion systems because we did not use the assumptions (A1)-(A3) concerning the gradient/skew-gradient structure.

In order to study the stability of the standing pulse ϕ, we have to compute (3.10). In general, we can not know any concrete informations about Ψ^* in (3.10), which is defined by the adjoint system (3.8). However, if (2.5) has the gradient/skew-gradient structure, we find that

$$\Psi^* = K\Phi = \begin{pmatrix} QD\phi''(x) \\ -QD\phi'(x) \end{pmatrix} \tag{3.11}$$

holds, where K is the skew-symmetric matrix defined by (2.8). Hence we can compute the Melnikov integral (3.10), which determines the linear stability of the standing pulse ϕ. (3.11) suggests that reaction-diffusion systems with the gradient/skew-gradient structure have symmetry in some sense.

§4. Stability analysis of spatially periodic stationary solutions

In this section, according to [5, 6], we consider the linear stability of spatially periodic stationary solutions of (2.5) with the gradient/skew-gradient structure. Let $\varphi(x;\ell)$ be a family of spatially periodic stationary solutions of (2.5) parameterized by its wavelength ℓ, that is,

$$D\varphi(x;\ell)_{xx} + f(\varphi(x;\ell)) = 0, \tag{4.1}$$

$$\varphi(x;\ell) = \varphi(x+\ell;\ell). \tag{4.2}$$

Notice that we do not require any other assumptions about $\varphi(x;\ell)$ such as smallness and symmetry. As seen in Section 2, $\Phi = (\varphi, \varphi_x)^T$ is a solution of the Hamiltonian system

$$K\Phi_x = -\nabla_Z H(\Phi), \tag{4.3}$$

where K is the skew-symmetric matrix defined by (2.8), and H is the first integral (Hamiltonian) given by (2.9). In order to study the linear stability of $\varphi(x;\ell)$, we are concerned with the linearized eigenvalue problem of (2.5) at $\varphi(x;\ell)$ defined by

$$\lambda T v = D v_{xx} + f_u(\varphi(x;\ell))v \tag{4.4}$$

on the space $L^2(\mathbf{R})$.

In what follows, we consider (4.4) by a formal argument based on the Floquet theory (Bloch transformation) and the analytic perturbation theory. As for a mathematical background of the following argument, the reader should consult [4, 12, 13] and the references theirin.

Setting $V = (v,\, v_x)^T$, we rewrite (4.4) as a first-order ODE

$$KV_x = S(x;\ell)V + \lambda N V, \tag{4.5}$$

where

$$S(x;\ell) = \begin{pmatrix} -\nabla^2 F(\varphi(x;\ell)) & 0 \\ 0 & -QD \end{pmatrix}, \quad N = \begin{pmatrix} QT & 0 \\ 0 & 0 \end{pmatrix}. \tag{4.6}$$

Let

$$L = K\frac{d}{dx} - S(x;\ell).$$

Then, we (formally) see that the first order differential operator L is self-adjoint because K and $S(x;\ell)$ are skew-symmetric and symmetric matrices, respectively. By using L, (4.5) is simply written as

$$LV = \lambda N V. \tag{4.7}$$

Applying the Bloch transformation $V = We^{ikx}$, we have

$$LW = \lambda N W - ikKW, \tag{4.8}$$

where $W \in L^2_{per}(0,\ell)$. According to [6], the self-adjoint operator L on $L^2_{per}(0,\ell)$ has the following property:

Lemma [6] Let $\psi_1 = \Phi_x$ and $\psi_2 = x\Phi_x + \ell\Phi_\ell$. Then, $\psi_1,\ \psi_2 \in L^2_{per}(0,\ell)$ and

$$L\psi_1 = 0 \quad \text{and} \quad L\psi_2 = K\psi_1 \tag{4.9}$$

hold, where $\Phi = (\varphi, \varphi_x)^T$.

We now solve (4.8) by using a simple perturbative argument. Suppose that λ and W in (4.8) can be expanded with respect to k around $k = 0$. Then it follows from (4.9) that $\lambda(0) = 0$ and $W(0) = \psi_1$. Differentiating (4.8) with respect to k, we have

$$LW_k = \lambda_k NW + \lambda NW_k - iKW - ikKW_k. \tag{4.10}$$

Setting $k = 0$, we have

$$LW_k = \lambda_k N\psi_1 - iK\psi_1.$$

Since L is self-adjoint, applying the solvability condition, we have

$$[\psi_1,\ \lambda_k N\psi_1 - iK\psi_1] = 0,$$

where $[\ ,\ ]$ denotes the usual inner product on $L^2_{per}(0,\ell)$. Recalling that ψ_1 is real, and that K is skew-symmetric, we have

$$\lambda_k = \frac{i[\psi_1,\ K\psi_1]}{[\psi_1,\ N\psi_1]} = 0,$$

which implies $LW_k = -iK\psi_1$. Comparing this result with the second equation of (4.9), we obtain

$$W_k = -i\psi_2.$$

Similarly, differentiating (4.10) with respect to k, and setting $k = 0$, we have

$$LW_{kk} = \lambda_{kk} N\psi_1 - 2K\psi_2.$$

Hence, applying the solvability condition, we obtain

$$\lambda_{kk} = \frac{2[\psi_1,\ K\psi_2]}{[\psi_1,\ N\psi_1]}.$$

Since K is skew-symmetric, by using (2.8), (4.6) and (4.3), a direct calculation shows that

$$[\psi_1,\ N\psi_1] = \int_0^\ell \langle T\varphi_x,\ Q\varphi_x\rangle dx := I(\ell),$$

$$[\psi_1,\ K\psi_2] = [\Phi_x,\ xK\Phi_x] + \ell[\Phi_x,\ K\Phi_\ell] = \ell[-K\Phi_x,\ \Phi_\ell]$$

$$= \ell[\nabla_Z H(\Phi),\ \Phi_\ell] = \ell^2 \cdot \frac{dH(\ell)}{d\ell},$$

where

$$H(\ell) = \frac{1}{2}\langle D\varphi_x, Q\varphi_x\rangle + F(\varphi) \tag{4.11}$$

is a first integral (Hamiltonian) which is independent of x (cf. (2.9)). Therefore, we obtain

$$\lambda = \lambda(k) = \frac{\ell^2}{I(\ell)}\frac{dH(\ell)}{d\ell}k^2 + O(k^3) \tag{4.12}$$

for sufficiently small k. Thus we see that $\lambda > 0$ holds if $I(\ell)$ and $H'(\ell)$ have same signs, so that $\varphi(x;\ell)$ is linearly unstable if $I(\ell)$ and $H'(\ell)$ have same signs.

As seen in the above argument, the linear (in)stability of $\varphi(x;\ell)$ is due to perturbations having a large spatial period. It is known as the Eckhaus instability [2] which was originally obtained in the study of the linear stability of roll patterns in thermal convection phenomena.

§5. Concluding remarks

As we have observed in the arguments so far, the notion of gradient/skew-gradient structure enables us to use the Hamiltonian formalism for studying pattern formation problems in reaction-diffusion systems. The approach explained in this survey is quite natural because it is extensively used in the study of dynamics of a fluid and a motion of rigid bodies [1, 7, 8, 9].

In our knowledge, there are not so many works concerning reaction-diffusion systems with the gradient/skew-gradient structure. Especially, in higher dimensional cases, there has been no results yet except [15]. Recently, singular perturbation problems in reaction-diffusion systems can be treated under the gradient/skew-gradient structure [3]. We expect that the it gives an useful viewpoint for studying pattern formation problems in reaction-diffusion systems.

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