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Shadow system for adsorbate-induced phase transition model

Dedicated to Professor Toshitaka Nagai on the occasion of his sixtieth birthday

By

Kousuke KUTO * and Tohru TSUJIKAWA **

Abstract

Hildebrand et al. [6] proposed a kinematic model describing a structural phase transition arising in surface chemistry. By the numerical simulations, several stationary patterns of this model are shown in [17]. In the present paper, we introduce a *shadow system* in a limiting case that a diffusion coefficient tends to infinity and show the bifurcation structure of stationary solutions of the system in the one-dimensional case.

§ 1. Introduction

Nonequilibrium chemical reactions provide many interesting phenomena as complex spatiotemporal patterns, including target, spiral waves and wave turbulence. In contrast to this reaction, the catalytic surface reaction of CO oxidation on the platinum display the same basic patterns and new spatiotemporal pattern of standing waves [7]. The characteristic length scales of such patterns lay in the range of tens of micrometers, whereas the diffusion length of the mobile adsorbated particles. Therefore, these patterns were effectively macroscopic and their properties could well be described by the classical reaction-diffusion equation [1], [8]. However, it was experimentally shown

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*Department of Intelligent Mechanical Engineering, Fukuoka Institute of Technology, Fukuoka, 811-0295, Japan.
e-mail: kuto@fit.ac.jp
**Department of Applied Physics, University of Miyazaki, Miyazaki, 889-2192, Japan.
e-mail: tujikawa@cc.miyazaki-u.ac.jp

the evidence of a great variety of the patterns on spatiotemporal sub and nanomicrometer scales [20]. Since these structures is on the scales shorter than the diffusion length, which is the mean distance passed by adsorbated particles, such reaction diffusion equation can not explain the mechanism of these pattern formations. Then it was introduced another mechanism leading to the formation of reactive nanostructures which involves adsorbate-induced structural phase transitions on the metal substrate. There are several models resulting from the interplay between the reaction, diffusion, and an adsorbate-induced structural transformation of the surface [6], [5], [4], [2], [13].

In this paper, we consider the following model proposed by Hildebrand [4]:

$$
\text{(P)} \quad \begin{cases} u_t = d\Delta u + u(1-u)(u+v-1) & \text{in } \ \Omega \times (0,\infty), \\ v_t = D\Delta v + \gamma\nabla\cdot\{v(1-v)\nabla\chi(u)\} + g(u,v) & \text{in } \ \Omega \times (0,\infty), \\ \dfrac{\partial u}{\partial \nu} = \dfrac{\partial v}{\partial \nu} = 0 & \text{on } \ \partial\Omega \times (0,\infty), \\ u(\,\cdot\,,0) = u_0, \quad v(\,\cdot\,,0) = v_0 & \text{in } \ \Omega, \end{cases}
$$

where Ω is a bounded domain in $\boldsymbol{R}^n$ $(n = 1,2)$ with the boundary $\partial\Omega$ and d, D, γ are positive constants. The unknown functions $u = u(x,t)$ and $v = v(x,t)$ denote the structural state of surface and the adsorbate coverage rate of the surface by CO molecules at a position $x \in \Omega$ and time $t \in [0,\ \infty)$, respectively. The functions $\chi(u)$ and $g(u,v)$ are defined by

$$
\chi(u) = u^2(2u-3), \quad g(u,v) = c(1-v) - ae^{\alpha\chi(u)}v - bv, \tag{1.1}
$$

where $a,\ b,\ c$ and α are positive constants. As shown in Tsujikawa, Yagi [19], Takei et al. [16], [17], there exists a unique global solution of (P) for $n = 2$ and an exponential attractor of the corresponding dynamical system.

From the view point of the pattern formation, it is important to consider the existence of the stationary solutions and their stability. Hildebrand et al. [6], [5] and Tsujikawa [18] show the existence of standing pulse solutions and their stability in $\boldsymbol{R}$ and $\boldsymbol{R}^2$ as $d \to 0$, by using the singular perturbation method. On the other hand, various types of stationary patterns by numerical computations in [13], [17] are obtained. They are stationary stripe, square and hexagonal patterns on the surface and we show the existence of the corresponded stationary solutions by the bifurcation theory [9], which implies the local structure near the bifurcation point. Furthermore in [10] we have obtained the sufficient conditions on d for the existence or nonexistence of nonconstant stationary solutions of (P).

In the present paper, we focus on the limiting profiles of stationary patterns as $D \to \infty$. Our limiting analysis is to study a *shadow system* by setting $D \to \infty$ in the stationary problem of (P). The reason why we study the shadow system is that solutions of the shadow system may perturb stationary patterns of the original system (P) in a situation when the motility D of CO molecules is very large. Namely, any sequence of stationary patterns of (P) with $D = D_n$ approaches a positive solution of the shadow system as $D_n \to \infty$ passing to a subsequence. Our purpose of this paper is to derive much information on the global bifurcation structure of non-constant solutions to the shadow system in 1-dimensional case.

The organization of this paper is as follows. In Section 2 we introduce the shadow system corresponding to the stationary problem of (P) in the limiting case $D \to \infty$ and show the existence of non-constant solutions in some parameter region of $(d,\ a,\ b,\ c,\ \alpha)$. Finally, in Section 3 we discuss the dependency of the non-constant solutions on these parameters by the numerical computations.

§ 2. Shadow system

In 1-dimensional case, the stationary problem of (P) is reduced to the following boundary value problem of ordinary differential equations:

$$\text{(SP)}\ \begin{cases} du'' + u(1-u)(u+v-1) = 0, & 0 < x < 1, \\ Dv'' + \gamma\{v(1-v)\chi_u(u)u'\}' + g(u,v) = 0, & 0 < x < 1, \\ u'(0) = u'(1) = 0, \quad v'(0) = v'(1) = 0. \end{cases}$$

Here '$'$' denotes the derivative with respect to x. By the modelling aspect, we are restricted on non-negative solutions. Hence the maximal principle implies that for any non-constant solution $(u, v) \geq 0$ satisfies

$$0 < u(x) < 1 \quad \text{for} \quad 0 \leq x \leq 1. \tag{2.1}$$

Furthermore, in a forthcoming paper [10] we obtain a uniform bound $M > 0$ such that

$$\|(u,v)\|_{H^2} \leq M \tag{2.2}$$

for any positive solution (u, v) of (SP).

In the present paper, we study the qualitative behaviour of solutions of (SP) in a limiting case $D \to \infty$. Let (u_D, v_D) be any positive solution of (SP). Then thanks to (2.2), a standard compactness argument enables us to find a subsequence $\{(u_{D_j}, v_{D_j})\} \subset \{(u_D, v_D)\}$ as $D = D_j \to \infty$ such that

$$\lim_{j\to\infty}(u_{D_j}, v_{D_j}) = (u_\infty, v_\infty) \quad \text{in} \quad H^1(0,1) \times H^1(0,1). \tag{2.3}$$

Since (2.3) leads to $v''_\infty = 0$ by letting $D_j \to \infty$ in the weak form of (SP), then one can verify

$$v_\infty = \theta$$

is a constant from the boundary condition. Therefore, integrating the second equation of (SP) on the interval, we have the following *shadow system* which (u_∞, θ) satisfies:

$$\text{(SS)} \begin{cases} du'' + u(1-u)(u+\theta-1) = 0, \quad 0 < x < 1, \\ u'(0) = u'(1) = 0, \\ \displaystyle\int_0^1 g(u,\theta)\ \mathrm{d}x = 0. \end{cases}$$

Our aim is to obtain the set of non-constant positive solutions of (SS). To do so, we first regard θ as a given parameter and study the boundary value problem of an Allen-Cahn type equation:

$$\begin{cases} du'' + u(1-u)(u+\theta-1) = 0, \quad 0 < x < 1, \\ u'(0) = u'(1) = 0. \end{cases} \tag{2.4}$$

Our strategy of analysis for (SS) is to choose a solution (u, θ) matching the integral condition

$$\int_0^1 g(u,\theta)\ \mathrm{d}x = 0 \tag{2.5}$$

in the set of positive solutions of (2.4). Here we remark that (1.1) and (2.5) imply

$$0 < \theta < 1.$$

§ 2.1. Bifurcation structure of solutions of (2.4)

In what follows, we regard d as a bifurcation parameter. Thanks to 1-dimensional case, for each $\theta \in (0,1)$, we have only to study the set of monotone increasing solutions

$$\Gamma(\theta) = \big\{(u,d) \in C^2([0,1]) \times \boldsymbol{R}_+ \,|\, u \text{ is a positive solution of (2.4) with } u' > 0 \text{ in } (0,1)\big\}$$

because any positive solution can be constructed by suitable rescaling and reflections of some $(u,d) \in \Gamma(\theta)$. For example, the set of monotone decreasing positive solutions can be represented by $\{(u_-, d) \,|\, (u,d) \in \Gamma(\theta)\}$ with $u_-(x) := u(1-x)$; the set of 4-mode positive solutions can also be represented by

$$\{(\tilde{u}, d/4^2) \,|\, (u,d) \in \Gamma(\theta)\} \cup \{(\tilde{u}_-, d/4^2) \,|\, (u,d) \in \Gamma(\theta)\},$$

where

$$\tilde{u}(x) := \begin{cases} u(4x) & \text{for } \ x \in [0, \frac{1}{4}], \\ u(4(\frac{1}{2} - x)) & \text{for } \ x \in [\frac{1}{4}, \frac{1}{2}], \\ u(4(x - \frac{1}{2})) & \text{for } \ x \in [\frac{1}{2}, \frac{3}{4}], \\ u(4(1-x)) & \text{for } \ x \in [\frac{3}{4}, 1]. \end{cases}$$

Smoller and Wasserman [15] obtained the following branch of $\varGamma(\theta)$ bifurcating from the constant solution $u = 1 - \theta$ at

$$d^* = \frac{\theta(1-\theta)}{\pi^2}.$$

Lemma 2.1 ([15]). *The set $\varGamma(\theta)$ bifurcates from the constant solution $u = 1-\theta$ at $d = d^*$ and forms a bounded smooth curve with respect to $d \in (0, d^*)$. Then for each $d \in (0, d^*)$, $\varGamma(\theta)$ possesses a unique element $u(\,\cdot\,, d)$ and*

$$d \to u(\,\cdot\,, d) \,:\, (0, d^*) \to C^2([0,1])$$

is a continuous mapping with

$$\lim_{d \to d^*} u(\,\cdot\,, d) = 1 - \theta \quad \textit{in} \quad C^2([0,1]).$$

Furthermore, the following behaviours of $(u(\,\cdot\,,d), d) \in \varGamma(\theta)$ as $d \to 0$ are satisfied according to two cases (i) $0 < \theta < 1/2$ *and* (ii) $1/2 < \theta < 1$.

(i) *In case $0 < \theta < 1/2$, define $\zeta > 0$ by*

$$\int_\zeta^1 u(1-u)(u+\theta-1)\,\mathrm{d}u = 0.$$

In this case, $u(\,\cdot\,,\, d) \in \varGamma(\theta)$ satisfies

$$\lim_{d \to 0} u(x,d) = \begin{cases} \zeta & \textit{for} \quad x = 0, \\ 1 & \textit{for} \quad x \in (0,1], \end{cases}$$

and moreover,

$$\lim_{d \to 0} u(\,\cdot\,, d) = 1 \quad \textit{uniformly on any compact subset of } (0,1).$$

(ii) *In case $1/2 < \theta < 1$, define $\eta > 0$ by*

$$\int_0^\eta u(1-u)(u+\theta-1)\,\mathrm{d}u = 0.$$

In this case, $u(\,\cdot\,,\, d) \in \varGamma(\theta)$ satisfies

$$\lim_{d \to 0} u(x,d) = \begin{cases} 0 & \textit{for} \quad x \in [0,1), \\ \eta & \textit{for} \quad x = 1, \end{cases}$$

and moreover,

$$\lim_{d \to 0} u(\,\cdot\,, d) = 0 \quad \textit{uniformly on any compact subset of } (0,1).$$

We will obtain the set of monotone increasing solutions of (SS). In order to find positive solutions of (SS) in $\varGamma(\theta)$, we regard θ as a parameter and denote monotone increasing functions in $\varGamma(\theta)$ by

$$u(x, d, \theta). \tag{2.6}$$

By virtue of Lemma 2.1, we set the domain of the mapping $(d, \theta) \mapsto u(\,\cdot\,, d, \theta)$ by the union of

$$\mathcal{A} := \left\{ (d, \theta) \,:\, 0 < d < \frac{\theta(1-\theta)}{\pi^2} =: d^*(\theta),\ 0 < \theta < \frac{1}{2} \right\}$$

and

$$\mathcal{B} := \left\{ (d, \theta) \,:\, 0 < d < \frac{\theta(1-\theta)}{\pi^2} =: d^*(\theta),\ \frac{1}{2} < \theta < 1 \right\}.$$

Then Lemma 2.1 implies the mapping

$$(d, \theta) \mapsto u(\,\cdot\,, d, \theta) \,:\, \mathcal{A} \cup \mathcal{B} \to C^2([0, 1]) \tag{2.7}$$

is continuous.

Our aim is to construct the set of (d, θ) such that $u(x, d, \theta)$ satisfies the integral condition (2.5). It follows from (1.1) that (2.5) is reduced to

$$\left(a \int_0^1 e^{\alpha\chi(u)}\, \mathrm{d}x + b + c \right) \theta = c. \tag{2.8}$$

By virtue of (2.8), we define a mapping

$$\varPhi(d, \theta) = \left(a \int_0^1 e^{\alpha\chi(u(x,d,\theta))}\, \mathrm{d}x + b + c \right) \theta \tag{2.9}$$

for every $u(\,\cdot\,, d, \theta) \in \varGamma(\theta)$. It follows from (2.7) and (2.9) that

$$(d, \theta) \mapsto \varPhi(d, \theta) \,:\, \mathcal{A} \cup \mathcal{B} \to \boldsymbol{R}$$

yields a continuous mapping. We will find $(d, \theta) \in \mathcal{A} \cup \mathcal{B}$ with

$$\varPhi(d, \theta) = c \tag{2.10}$$

to obtain the set of monotone increasing solutions of (SS).

§ 2.2. Matching the integral condition : Case of $0 < \theta < 1/2$

We will design the solution set of (2.10) in $\mathcal{A}$. From (2.9) and (i) of Lemma 2.1, we immediately obtain the following profile of $\varPhi(d, \theta)$ as $d \to 0$ and $d \to d^*(\theta)$:

Lemma 2.2. *For any* $\theta \in (0, 1/2)$,

$$\Phi(0,\theta) := \lim_{d \to 0} \Phi(d,\theta) = (ae^{-\alpha} + b + c)\theta$$

and

$$\Phi(d^*(\theta),\theta) := \lim_{d \to d^*(\theta)} \Phi(d,\theta) = (ae^{\alpha\chi(1-\theta)} + b + c)\theta.$$

Then by (1.1),

$$\Phi(0,\theta) < \Phi(d^*(\theta),\theta) \quad \text{for} \quad \theta \in \left(0, \frac{1}{2}\right). \tag{2.11}$$

With use of Lemma 2.2, we solve $\Phi(d,\theta) = c$ in $\mathcal{A}$ to get the solution set of (SS) when $0 < \theta < 1/2$.

Theorem 2.3. *Suppose that* $c < ae^{-\alpha/2} + b$. *There exist* $0 < \underline{\theta} < \overline{\theta} \leq 1/2$ *such that for any* $\theta \in (\underline{\theta}, \overline{\theta})$, (SS) *has a monotone increasing positive solution* $u(x, d(\theta), \theta) \in \Gamma(\theta)$ *for some positive number* $d = d(\theta)$. *More precisely,* $d(\theta)$ *is a lower semi-continuous function in* $(\underline{\theta}, \overline{\theta})$ *with* $d(\underline{\theta}) = d^*(\underline{\theta})$ *and the following properties*:

(i) *If* $c < ae^{-\alpha} + b$, *then* $\overline{\theta} < 1/2$, $d(\overline{\theta}) = 0$,

$$\lim_{\theta \to \overline{\theta}} u(x, d(\theta), \theta) = 1 \quad \text{for} \quad x \in (0, 1]$$

and

$$u(\,\cdot\,, d(\underline{\theta}), \underline{\theta}) = 1 - \underline{\theta}.$$

(ii) *If* $ae^{-\alpha} + b < c < ae^{-\alpha/2} + b$, *then* $\overline{\theta} = 1/2$ *and* $u(\,\cdot\,, d(\underline{\theta}), \underline{\theta}) = 1 - \underline{\theta}$.

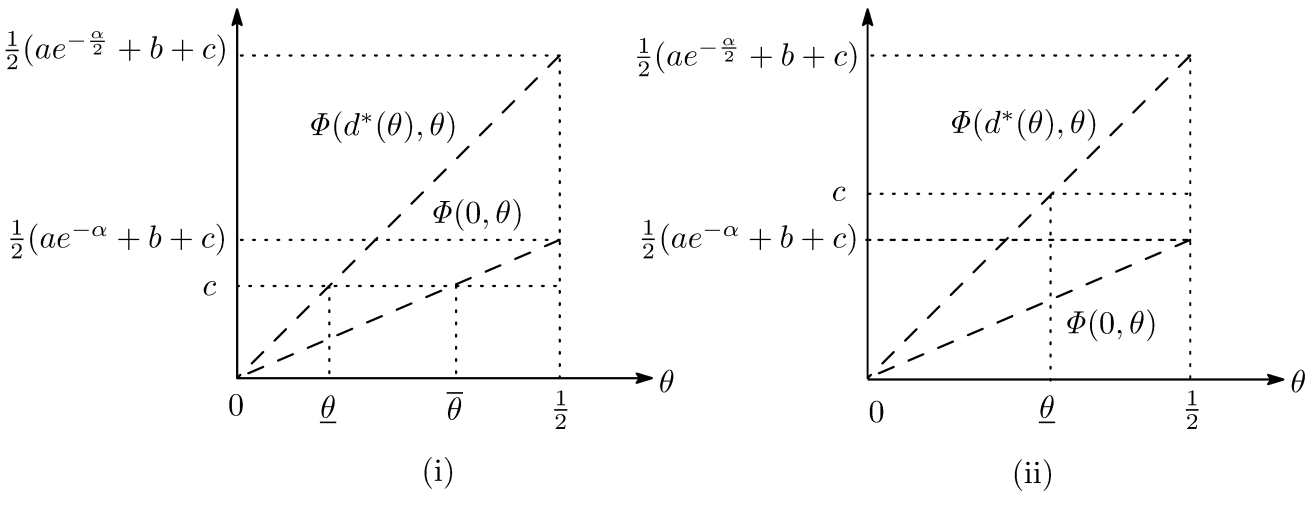

Figure 1

Proof. To construct the level set of $\Phi(d,\theta)=c$, we study the family of continuous curves

$$\{\Phi(d,\theta)\,:\,(d,\theta)\in\mathcal{A}\}.$$

In view of (1.1) and Lemma 2.2, we know that both

$$\Phi(0,\theta)=(ae^{-\alpha}+b+c)\theta\quad\text{and}\quad\Phi(d^*(\theta),\theta)=(ae^{\alpha\chi(1-\theta)}+b+c)\theta$$

are monotone increasing for $\theta\in(0,1/2)$ and satisfy (2.11). Furthermore Lemma 2.2 yields the liming behaviours of $\Phi(0,\theta)$ and $\Phi(d^*(\theta),\theta)$ as $\theta\to1/2$ and $\theta\to0$;

$$\lim_{\theta\to1/2}\Phi(0,\theta)=\frac{ae^{-\alpha}+b+c}{2}<\lim_{\theta\to1/2}\Phi(d^*(\theta),\theta)=\frac{ae^{-\alpha/2}+b+c}{2}\tag{2.12}$$

and

$$\lim_{\theta\to0}\Phi(0,\theta)=\lim_{\theta\to0}\Phi(d^*(\theta),\theta)=0.\tag{2.13}$$

We first discuss the case when

$$c<\lim_{\theta\to1/2}\Phi(0,\theta)=\frac{ae^{-\alpha}+b+c}{2},\tag{2.14}$$

that is, $c<ae^{\alpha/2}+b$. In this case, it follows from (2.13) and (2.14) that the intermediate theorem ensures $0<\overline{\theta}<1/2$ such that

$$\Phi(0,\overline{\theta})=c.$$

Here we remark that such a number $\overline{\theta}$ is uniquely determined by the monotonicity of $\theta\mapsto\Phi(0,\theta)$. Since $c<\lim_{\theta\to1/2}\Phi(d^*(\theta),\theta)$ by (2.12) and (2.14), one can use the intermediate theorem again for the monotone function $\theta\mapsto\Phi(d^*(\theta),\theta)$ to find a unique number $0<\underline{\theta}<1/2$ such that

$$\Phi(d^*(\underline{\theta}),\underline{\theta})=c.$$

Consequently, by virtue of (2.11), we have obtained $0<\underline{\theta}<\overline{\theta}<1/2$ such that

$$\Phi(d^*(\underline{\theta}),\underline{\theta})=c\quad\text{and}\quad\Phi(0,\overline{\theta})=c\tag{2.15}$$

when $c<ae^{\alpha/2}+b$. Then in this case, (2.15) and the monotone increasing properties of $\theta\mapsto\Phi(0,\theta)$ and $\theta\mapsto\Phi(d^*(\theta),\theta)$ yield

$$\Phi(0,\theta)<c<\Phi(d^*(\theta),\theta)\quad\text{for}\quad\theta\in(\underline{\theta},\overline{\theta}).$$

Therefore, for any fixed $\theta_0\in(\underline{\theta},\overline{\theta})$, the intermediate theorem for the continuous function $\Phi(d,\theta)$ ensures at least one positive number d_0 such that $\Phi(d_0,\theta_0)=c$. Then for $\theta\in(\underline{\theta},\overline{\theta})$, we can define a positive function $d(\theta)$ by

$$d(\theta):=\inf\{d>0\,:\,\Phi(d,\theta)=c\}.$$

Hence $d(\theta)$ forms a lower semi-continuous function in $(\underline{\theta}, \overline{\theta})$. Additionally in view of (2.15), we set

$$d(\underline{\theta}) = d^*(\underline{\theta}) \quad \text{and} \quad d(\overline{\theta}) = 0. \tag{2.16}$$

Obviously $u(x, d(\theta), \theta) \in \Gamma(\theta)$ satisfies the integral condition (2.5) and becomes a monotone increasing solution of (SS). Owing to Lemma 2.1 and the continuity of (2.7), we can use (2.16) to derive the limiting behaviours in (i) of Theorem 2.3 by letting $\theta \to \underline{\theta}$ and $\theta \to \overline{\theta}$ in $u(\,\cdot\,, d(\theta), \theta)$.

By virtue of (2.11), we study the case

$$\lim_{\theta \to 1/2} \Phi(0, \theta) = \frac{ae^{-\alpha} + b + c}{2} < c < \lim_{\theta \to 1/2} \Phi(d^*(\theta), \theta) = \frac{ae^{-\alpha/2} + b + c}{2},$$

that is,

$$ae^{-\alpha} + b < c < ae^{-\alpha/2} + b.$$

Hence the intermediate theorem for the monotone function $\theta \mapsto \Phi(d^*(\theta), \theta)$ gives a unique $\underline{\theta} \in (0, 1/2)$ such that

$$\Phi(d^*(\underline{\theta}), \underline{\theta}) = c.$$

Along a similar argument to the above case, the continuity of $\Phi(d, \theta)$ enables us to find a lower semi-continuous function $d = d(\theta)$ for $\theta \in (\underline{\theta}, 1/2)$ such that

$$\Phi(d(\theta), \theta) = c \quad \text{for} \quad \theta \in \left(\underline{\theta}, \frac{1}{2}\right) \quad \text{with} \quad d(\underline{\theta}) = d^*(\underline{\theta}). \tag{2.17}$$

It follows from Lemma 2.1 and the continuity of (2.7) that (2.17) ensures the assertion (ii) of Theorem 2.3. $\square$

Remark 2.4. Through the analysis for the balanced case $\theta = 1/2$, it is possible to prove $\lim_{\theta \to 1/2} d(\theta) = 0$ when $ae^{-\alpha} + b < c < ae^{-\alpha/2} + b$. We omit the proof because a similar argument is appeared in [11]. However it leaves an interesting open problem to reveal the singular limiting behaviour of $u(\,\cdot\,, d(\theta), \theta)$ as $d(\theta) \to 0$ $(\theta \to 1/2)$.

§ 2.3. Matching the integral condition : Case of $1/2 < \theta < 1$

For the case of $1/2 < \theta < 1$, (2.9) and (ii) of Lemma 2.1 give the following profile of $\Phi(d, \theta)$ in $\mathcal{B}$:

Lemma 2.5. *For any $\theta \in (1/2, 1)$,*

$$\Phi(0, \theta) := \lim_{d \to 0} \Phi(d, \theta) = (a + b + c)\theta$$

and

$$\Phi(d^*(\theta),\theta) := \lim_{d\to d^*(\theta)} \Phi(d,\theta) = (ae^{\alpha\chi(1-\theta)} + b + c)\theta.$$

Then by (1.1),

$$\Phi(0,\theta) > \Phi(d^*(\theta),\theta) \quad \textit{for} \quad \theta \in \left(\frac{1}{2}, 1\right). \tag{2.18}$$

In case of $1/2 < \theta < 1$, we obtain monotone increasing solutions of (SS) if $c > e^{-\alpha/2} + b$. This existence range gives a complement of that in the previous case $0 < \theta < 1/2$.

Theorem 2.6. *Suppose that $c > ae^{-\alpha/2} + b$. There exist $1/2 \le \underline{\theta} < \overline{\theta} < 1$ such that for any $\theta \in (\underline{\theta}, \overline{\theta})$,* (SS) *has a monotone increasing positive solution $u(x, d(\theta), \theta) \in \Gamma(\theta)$ for some positive number $d = d(\theta)$. More precisely, $d(\theta)$ is a lower semi-continuous function in $(\underline{\theta}, \overline{\theta})$ with $d(\overline{\theta}) = d^*(\overline{\theta})$ and the following properties*:

(i) *If $ae^{-\alpha/2} + b < c < a + b$, then $\underline{\theta} = 1/2$ and*

$$u(\,\cdot\,, d(\overline{\theta}), \overline{\theta}) = 1 - \overline{\theta}.$$

(ii) *If $a + b < c$, then $1/2 < \underline{\theta}$, $d(\underline{\theta}) = 0$,*

$$\lim_{\theta\to\underline{\theta}} u(x, d(\theta), \theta) = 0 \quad \textit{for} \quad x \in [0, 1)$$

and $u(\,\cdot\,, d(\overline{\theta}), \overline{\theta}) = 1 - \overline{\theta}$.

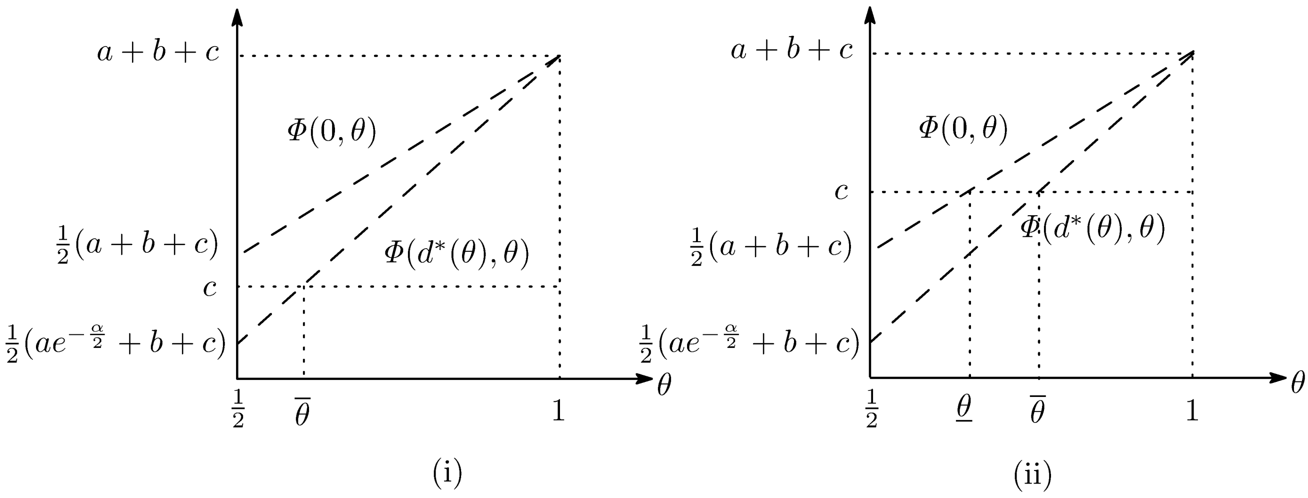

Figure 2

Proof. Suppose that $\theta \in (1/2, 1)$. As the proof of Theorem 2.3, we study the profiles of continuous curves

$$\{\Phi(d, \theta) \,:\, (d, \theta) \in \mathcal{B}\}$$

to construct the level set of $(d, \theta) \in \mathcal{B}$ with $\Phi(d, \theta) = c$. We remark that for any fixed $\theta \in (1/2, 1)$,

$$d \mapsto \Phi(d, \theta) \,:\, (0, d^*(\theta)) \to \boldsymbol{R}$$

forms a smooth function with (2.18). In view of Lemma 2.5, we know that

$$\Phi(0, \theta) = (a + b + c)\theta \quad \text{and} \quad \Phi(d^*(\theta), \theta) = (ae^{\alpha\chi(1-\theta)} + b + c)\theta$$

are monotone increasing functions with respect to $\theta \in (1/2, 1)$. Furthermore Lemma 2.5 yields the liming behaviours of $\Phi(0, \theta)$ and $\Phi(d^*(\theta), \theta)$ as $\theta \to 1/2$ and $\theta \to 1$;

$$\lim_{\theta \to 1/2} \Phi(0, \theta) = \frac{a + b + c}{2} > \lim_{\theta \to 1/2} \Phi(d^*(\theta), \theta) = \frac{ae^{-\alpha/2} + b + c}{2}$$

and

$$\lim_{\theta \to 1} \Phi(0, \theta) = \lim_{\theta \to 1} \Phi(d^*(\theta), \theta) = a + b + c > c.$$

Therefore, if

$$c > \frac{a + b + c}{2}, \quad \text{namely,} \;\; c > a + b,$$

then there exist

$$\frac{1}{2} < \underline{\theta} < \overline{\theta} < 1$$

such that

$$\Phi(0, \underline{\theta}) = c \quad \text{and} \quad \Phi(d^*(\overline{\theta}), \overline{\theta}) = c. \tag{2.19}$$

By the continuity of $\Phi(d, \theta)$, we can find a lower semi-continuous function $d = d(\theta)$ for $\theta \in (\underline{\theta}, \overline{\theta})$ such that

$$\Phi(d(\theta), \theta) = c.$$

Additionally, (2.19) implies

$$d(\underline{\theta}) = 0 \quad \text{and} \quad d(\overline{\theta}) = d^*(\overline{\theta}). \tag{2.20}$$

Therefore, we can show the assertion (ii) of Theorem 2.6 along the same argument in the proof of Theorem 2.3.

If c satisfies

$$\lim_{\theta \to 1/2} \Phi(0, \theta) = \frac{a + b + c}{2} > c > \lim_{\theta \to 1/2} \Phi(d^*(\theta), \theta) = \frac{ae^{-\alpha/2} + b + c}{2}$$

that is,

$$ae^{-\alpha/2} + b < c < a + b,$$

then there exists $\overline{\theta} \in (1/2, 1)$ such that

$$\Phi(d^*(\overline{\theta}), \overline{\theta}) = c.$$

Hence we obtain a lower semi-continuous function $d = d(\theta)$ for $\theta \in (1/2, \overline{\theta})$ such that

$$\Phi(d(\theta), \theta) = c \quad \text{for} \quad \theta \in \left(\frac{1}{2}, \overline{\theta}\right) \quad \text{with} \quad d(\overline{\theta}) = d^*(\overline{\theta}).$$

As the proof of Theorem 2.3, we get the assertion (i) of Theorem 2.6. □

Remark 2.7. As mentioned in Remark 2.4, with the aid of the analysis for the balanced case $\theta = 1/2$, we can prove that $\lim_{\theta \to 1/2} d(\theta) = 0$ when $ae^{-\alpha/2} + b < c < a + b$.

§ 3. Concluding Remarks

Summarizing Theorems 2.3 and 2.6, we have sufficient conditions for the existence of positive solutions as Table. In the model, c and θ represent the partial pressure of the molecules in the gas phase and the coverage rate of the surface by molecules, respectively. Then it may be said that our result in Table is reasonable, because the low (resp. high) coverage rate θ can be obtained for the low (resp. high) pressure c. However, our method does not give any information on existence or non-existence of non-constant positive solutions in the blank cases on Table.

	$0 < \theta < \frac{1}{2}$	$\frac{1}{2} < \theta < 1$
$a + b < c$		$\underline{\theta} < \theta < \overline{\theta}$
$ae^{-\alpha/2} < c < a + b$		$\frac{1}{2} < \theta < \overline{\theta}$
$ae^{-\alpha} + b < c < ae^{-\alpha/2} + b$	$\underline{\theta} < \theta < \frac{1}{2}$	
$c < ae^{-\alpha} + b$	$\underline{\theta} < \theta < \overline{\theta}$	

Table

By numerical computations, we obtain the bifurcation branches from the constant solution $u = 1 - \theta$, which corresponds to Theorems 2.3 and 2.6. Figures 3 and 4 imply that a monotone increasing solution is uniquely obtained for each $d > 0$ if it exists. Here, horizontal and vertical axes mean θ and d, respectively. When the branches arrive at the horizontal axis, the solution has a boundary layer for small $d > 0$.

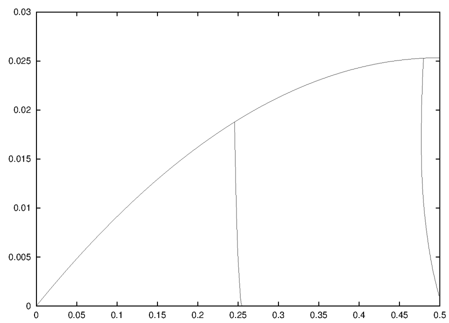

Figure 3

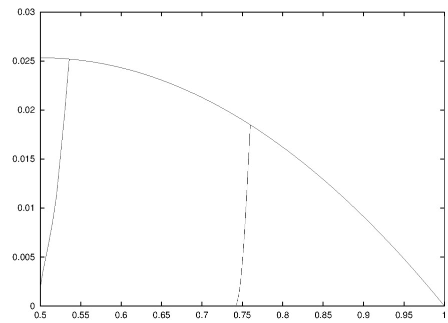

Figure 4

Figure 3: $a = 0.25, b = 0.2, \alpha = 1.0$. Left curve corresponds to the case (i) of Theorem 2.3, that is, $c = 0.1$, right curve corresponds to the case (ii), that is, $c = 0.32$.

Figure 4: $a = 0.25, b = 0.1, \alpha = 1.0$. Left curve corresponds to the case (i) of Theorem 2.6, that is, $c = 0.3$, right curve corresponds to the case (ii), that is, $c = 1.0$.

Figures 5 and 6 show the profiles of the function $c - \Phi(d, \theta)$ with respect to d in the cases corresponding to Figure 3 (ii) and Figure 4 (ii). From Figures 3, 4 and 5, we can find a non-monotone relationship (d, θ) of positive solutions $u(\cdot, d, \theta)$ of (SS). This result implies that there are two monotone increasing solutions with different diffusion coefficients for same θ.

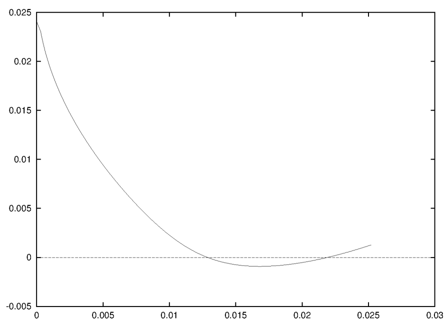

Figure 5

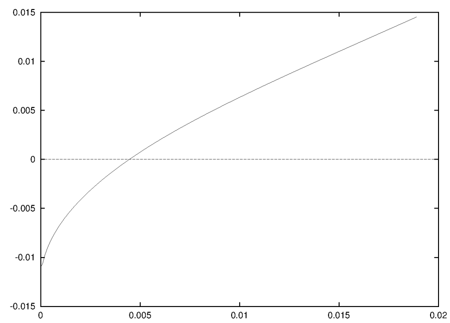

Figure 6

Figure 5: Parameters are same as the case of Figure 3 (ii) and $\theta = 0.478$.

Figure 6: Parameters are same as the case of Figure 4 (ii) and $\theta = 0.75$.

On the other hand, we can show the convergence of the solution of (SP) to the solution of (SS) in 1-dimensional case as $D \to \infty$ [10].

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