Condition for kink immobility in trigger systems with limited elimination of an inhibitor

A. A. Akhmetov
Department of Electronics, Kyushu University, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812, Japan
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Both the direction and the velocity of kink movement through a distributed trigger system depend on governing parameters that describe external factors affecting the system. Time and space scales for autocatalytic and inhibitory variables affect kink propagation as well. Coupled nonlinear one-dimensional equations were analyzed to estimate the difference in the governing parameters needed to stop a kink under conditions of zero and small but nonzero space scale for an inhibitory variable.

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Without the loss of generality, two dependent variables, autocatalytic $Y(\mathbf{r})$ and inhibitory $X(\mathbf{r})$, are needed for the proper description of the distributed trigger system [1]. Nonlinear diffusionlike equations with different time $T_{x(y)}$ and space $L_{x(y)}$ scales are to be written for both variables. If $T_x=0$ and $L_x=0$, the system can be reduced to one equation by eliminating X adiabatically. In the following we will use the term "submission" (of the inhibitory variable) as a synonym to the adiabatic elimination.

Distributed trigger systems of a different nature are characterized by two stable (basic) and one unstable stationary states which are uniform in space. Chemical reactors [1–3], normal metals at low temperatures [4], type-I superconductors [5–8], and composite superconductors [4,9] are known examples. The system undergoes transition from one basic state to the other when a switching wave (kink) moves along the system transforming it gradually in time. Under certain conditions the kink is an immobile boundary between the basic states [4,5,8–10]. Consider here the influence of a limited submission ($T_x \ll T_y, L_x \ll L_y$) of the inhibitory variable on the condition of the kink immobility. Corresponding one-dimensional equations can be written as

$$\tau\dot{X}=\epsilon X''+F_1(X,Y,\alpha)\ , \tag{1}$$

$$\dot{Y}=Y''+F_2(X,Y,\alpha)\ , \tag{2}$$

where

$$\tau=\frac{T_x}{T_y},\quad \epsilon=\left[\frac{L_x}{L_y}\right]^2$$

and α is a parameter describing external factors affecting the system (governing parameter). Solutions

$$Y=f_1(X,\alpha)\ , \tag{3}$$

$$Y=f_2(X,\alpha)\ , \tag{4}$$

of implicit equations

$$F_1(X,Y,\alpha)=0\ , \tag{5}$$

$$F_2(X,Y,\alpha)=0\ , \tag{6}$$

are known as null clines [1]. In the case of trigger systems, dependences given by Eqs. (3) and (4) have three points of intersection X_ι, Y_ι, $\iota=1,2,3$ corresponding to uniform stationary states. The autocatalytic variable null cline, $Y=f_2(X,\alpha)$, is S shaped (see Fig. 1). Nevertheless, the functions $X=\varphi_1(Y,\alpha)$ and $\varphi_2(Y,\alpha)$ which are inverse to the functions $f_1(X,\alpha)$ and $f_2(X,\alpha)$, respectively, are well defined.

If the kink is immobile, we can neglect the dependences of variables on time. Then, in the case $\epsilon=0$, Eqs. (1) and (2) are to be combined in

$$Y''+\Phi(Y,\alpha)=0\ , \tag{7}$$

where

$$\Phi(Y,\alpha)=F_2(Y,\varphi_1(Y,\alpha),\alpha)\ .$$

There are three points Y_ι for which

$$\Phi(Y_\iota,\alpha)=0\ . \tag{8}$$

Equation (8) describes the movement of a particle of unit mass in a given potential

$$S(Y,\alpha)=\int_{Y_1}^{Y_3}\Phi(Y,\alpha)dY\ . \tag{9}$$

Its solution, corresponding to the case when the particle begins its movement in the point $Y=Y_1$ with zero velocity and finishes its movement in the point $Y=Y_3$ with zero velocity as well, can be obtained if

$$S(Y_3,\alpha)=0\ . \tag{10}$$

Also Eq. (10) gives the condition for the kink immobili-

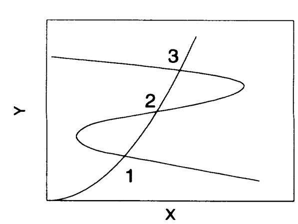

FIG. 1. Typical null clines for trigger system [1].

ty [4]. Together with Eq. (8) it defines the unique value α_c. At $\alpha=\alpha_c$ the shape of the immobile switching wave is given in implicit form as

$$z=\zeta(Y,\alpha_c),\quad \zeta(Y,\alpha_c)=\int_{Y_0}^{Y}\frac{dY}{\sqrt{-2S(Y,\alpha_c)}}\ , \tag{11}$$

where z is coordinate and $Y_1<Y_0<Y_3$, $z(Y_0)=0$ is an arbitrary value. If $\xi(z,\alpha_c)$ is an inverse function with respect to $\zeta(Y,\alpha_c)$, then the dependence of the inhibitory variable on coordinate is

$$X=\varphi_1(\xi(z,\alpha_c),\alpha_c)\ . \tag{12}$$

If the scale $\epsilon\neq 0$, $\epsilon\ll 1$, the dependence of the inhibitory variable on the autocatalytic variable changes slightly to match Eq. (1). Neglecting dependence on time, it follows

$$\epsilon\left[\frac{d^2}{dz^2}\varphi_1(\xi(z,\alpha_c),\alpha_c)\right]+F_1(X,Y,\alpha_c)=0\ . \tag{13}$$

Using Eq. (11), the expression enclosed in brackets can be written as a certain function of Y, i.e.,

$$\epsilon\Psi(Y,\alpha_c)+F_1(X,Y,\alpha_c)=0\ , \tag{14}$$

where

$$\Psi(Y)=-\left[2S(Y)\frac{d^2\varphi_1(Y)}{dY^2}+\Phi(Y)\frac{d\varphi_1(Y)}{dY}\right]\ . \tag{15}$$

For the sake of simplicity in the equations given here, and in the following, we only assume dependence on parameter α.

Using Eq. (14) and considering an alteration of the function $\varphi_1(Y)$ due to the presence of the nonzero parameter ϵ as variation, it follows

$$\varphi_1^{(\epsilon)}(Y)\approx\varphi_1(Y)-\epsilon\Psi(Y)\left[\frac{\partial F_1}{\partial X}\right]^{-1}\ , \tag{16}$$

where $\varphi_1^{(\epsilon)}$ represents the dependence of X on Y under the conditions of limited submission, and

$$\frac{\partial F_1}{\partial X}\equiv\left.\frac{\partial F_1(X,Y)}{\partial X}\right|_{X=\varphi_1(Y)}\ .$$

The corresponding variation of the function $\Phi(Y)$ due to the limited submission, i.e.,

$$\delta\Phi(Y)\equiv\Phi^{(\epsilon)}(Y)-\Phi(Y)\ ,$$

can be written as

$$\delta\Phi(Y)\approx-\epsilon\Psi(Y)\frac{\partial F_2}{\partial X}\left[\frac{\partial F_1}{\partial X}\right]^{-1}\ , \tag{17}$$

where

$$\frac{\partial F_2}{\partial X}\equiv\left.\frac{\partial F_2(X,Y)}{\partial X}\right|_{X=\varphi_1(Y)}\ .$$

A variation in $\Phi(Y)$ produces an alteration of the potential S in the point Y_3

$$\Delta S^{(\epsilon)}\approx\int_{Y_1}^{Y_3}\delta\Phi(Y)dY\ . \tag{18}$$

To return to the condition of the kink immobility $S(Y_3)=0$, it is necessary to change the governing parameter by the value $\Delta\alpha$ and by this produce a corresponding alteration of the potential S in the point Y_3

$$\Delta S^{(\alpha)}\approx\Delta\alpha\int_{Y_1}^{Y_3}\left.\frac{\partial\Phi(Y,\alpha)}{\partial\alpha}\right|_{\alpha=\alpha_c}dY\ . \tag{19}$$

The kink is immobile if

$$\Delta S^{(\epsilon)}+\Delta S^{(\alpha)}=0\ , \tag{20}$$

and substituting Eq. (15) we find that the alteration in the governing parameter needed to stop the kink under the condition of limited submission is

$$\Delta\alpha\approx-\epsilon\int_{Y_1}^{Y_3}\frac{\partial F_2}{\partial X}\left[\frac{\partial F_1}{\partial X}\right]^{-1}\left[2S\frac{\partial^2\varphi_1}{\partial Y^2}+\Phi\frac{\partial\varphi_1}{\partial Y}\right]dY\times\left[\int_{Y_1}^{Y_3}\left.\frac{\partial\Phi}{\partial\alpha}\right|_{\alpha=\alpha_c}dY\right]^{-1}\ . \tag{21}$$

Equation (21) though cumbersome in itself, allows us to avoid the time consuming dynamic calculation of the kink propagation in the trigger system described by two diffusionlike equations. Note that, given immobility of the kink, Eq. (21) is formally correct for any ratio of T_x and T_y. Condition $\tau\ll 1$ was chosen for avoiding the problem of kink instability due to a front bifurcation [10].

One of the simplest examples of a distributed trigger system is given by the equations of Belousov-Zhabotinskii chemical reaction written in the form [1] which contain not one but a few parameters governing the functions

$$F_1=Y(1-VX)-\gamma X\ , \tag{22}$$

$$F_2=\beta Y(1-X)-\frac{PY-\kappa}{qY+\eta}X-CY^2\ . \tag{23}$$

Considering the case of a full submission, $\epsilon=0$, it follows

$$\varphi_1(Y,V,\gamma)=\frac{Y}{YV+\gamma}\ , \tag{24}$$

and

$$\Phi=\beta Y\frac{Y(V-1)+\gamma}{VY+\gamma}-\frac{Y(PY-\kappa)}{(qY+\eta)(VY+\gamma)}-CY^2\ . \tag{25}$$

All integrations assumed in Eq. (21) can eventually be performed. However, for limits of the integration which are the roots of Eqs. (8) and (10) with function Φ given by Eq. (25), analytical expressions are too cumbersome. Because of this, simple numerical calculations were performed. It was found that for $\epsilon=0$ at $P=45$, $\beta=45$, $\gamma=0.01$, $\eta=0.5$, $q=8$, $\kappa=1$, and $C=1$, the kink is immobile when $V=1.1167$. Given these parameters, Eq. (21) was used to determine the changes in governing parameters V and C needed to stop the switching wave for the case of limited submission. The coefficient

$$K \equiv \frac{\Delta\alpha}{\epsilon}$$

was found to be

$$K = \begin{cases} +0.763 & \text{if } \alpha = C \\ -0.045 & \text{if } \alpha = V \,. \end{cases}$$

To verify applicability of Eq. (21) for the estimation of the conditions of kink immobility, Eqs. (1) and (2) for functions F_1 and F_2 given by Eqs. (22) and (23) were solved by FDM. At every set of parameters the boundary conditions corresponded to the stable stationary states. The length of the sample exceeded the largest scale of the problem many times.

First, Eqs. (8) through (11) were used to calculate the shape of the switching wave in the case $\epsilon = 0$. Then, the corresponding distribution $Y = Y(z, \alpha_c)$ was taken as an initial condition to study kink propagation. In accordance with previous results, the kink was immobile at $\alpha = \alpha_c$. The changing of the governing parameters lead to the alteration of the switching wave's form and to the kink movement towards one or the other end of the sample.

The next step was to introduce the small but nonzero parameter ϵ and to observe the kink movement in the media described by Eqs. (1) and (2) with boundary conditions $X = X_1$, $Y = Y_1$ on one side of the sample and $X = X_3$, $Y = Y_3$ on the other. By varying governing parameters it was possible to find the values V_c and C_c needed to stop the kink. The dependences of the values $\Delta V/\epsilon$ and $\Delta C/\epsilon$ on ϵ are shown in Fig. 2(a) and 2(b). It can be seen that at $\epsilon \rightarrow 0$ these dependences approach the values of the coefficient K calculated earlier.

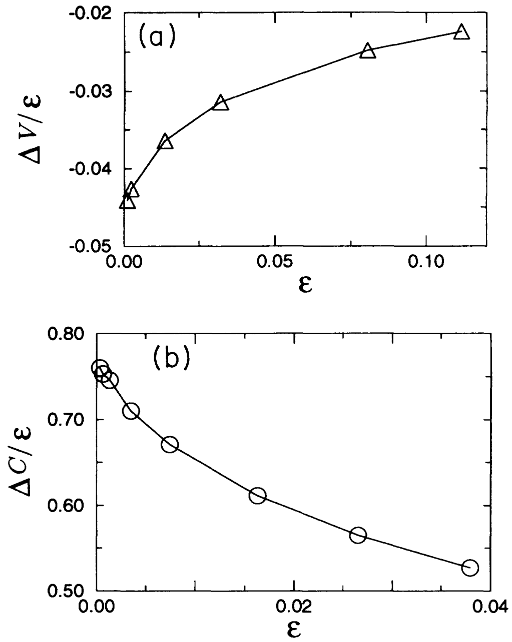

FIG. 2. Dependences of $\Delta\alpha$ on ϵ for the Belousov-Zhabotinskii chemical reaction: (a) $\alpha \equiv V$, (b) $\alpha \equiv C$.

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