

## Ultrafast Traveling Spike Autosolitons in Reaction-Diffusion Systems

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We have discovered a fundamentally new type of traveling wave solutions in reaction-diffusion systems—a traveling spike autosoliton. Using the proposed asymptotic method and the results of the numerical simulations, we investigated the shape of this autosoliton and the dependence of its basic characteristics on the system's parameters for the Brusselator. We have found that this autosoliton may have very large amplitude and velocity, and that its shape is in detailed qualitative agreement with that of the traveling pulses observed in the nerve tissue and in certain chemical reactions.

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One of the most picturesque phenomena in nonlinear physics lies in the fact that in certain homogeneous nonequilibrium systems one can excite steady localized patterns—autosolitons (AS) [1–3]. A typical example of an AS is a solitary wave propagating with constant speed  $v$  without decay—a traveling AS. Traveling AS are observed in many nonequilibrium systems, including heated electron-hole and gas plasmas, Belousov-Zhabotinsky reactions, and also in many biological systems, including cardiac and nerve tissue (see [1–7] and references therein).

The equations describing the kinetics of real systems far from equilibrium are extremely complicated. In order to investigate a traveling wave phenomena in such systems, Fitz-Hugh and Nagumo proposed a simplified model which consists of two coupled reaction-diffusion equations with a specific type of nonlinearity [8]. However, the shape of the traveling wave solutions realized in this model [9,10] is qualitatively different from those observed in the experiments on traveling waves in chemical reactions [11] and nerve tissue [7]. In this Letter we study the traveling wave solution in a system with a different type of nonlinearity and show that the shape of the pulse realized in this system is in detailed agreement with the experiments.

A rather general model of the nonequilibrium systems of interest is the set of two reaction-diffusion equations:

$$\tau_\theta \frac{\partial \theta}{\partial t} = l^2 \Delta \theta - q(\theta, \eta, A), \quad (1)$$

$$\tau_\eta \frac{\partial \eta}{\partial t} = L^2 \Delta \eta - Q(\theta, \eta, A), \quad (2)$$

where  $\theta$  is the activator, i.e., the variable with respect to which there is positive feedback;  $\eta$  is the inhibitor, i.e., the variable with respect to which there is negative feedback, and which controls the activator's growth; and  $A$  is the bifurcation parameter. Various examples of such systems were considered in Refs. [1–3] where the physics of activation and inhibition processes, as well as the meaning of the variables  $\theta$  and  $\eta$ , was discussed in detail.

In the general theory of AS [1,2] it was shown that, in the monostable systems described by Eqs. (1) and (2), traveling AS and more complex autowaves can be excited in the stability region of the homogeneous state when  $\alpha \equiv \tau_\theta / \tau_\eta \ll 1$  and  $\epsilon \equiv l/L \gtrsim \alpha$ . The theory of these AS is developed only for the case when the nullcline of Eq. (1), i.e., the dependence  $\eta(\theta)$  determined by the equation  $q(\theta, \eta, A) = 0$  for  $A = \text{const}$ , has N or inverted N form. In other words, for the given values of  $A$  and  $\eta$  the equation  $q(\theta, \eta, A) = 0$  has three solutions:  $\theta_h$ ,  $\theta_s$ , and  $\theta_{\max}$ . When  $\alpha \ll 1$  and  $\epsilon \gg 1$ , the front wall of the AS is a wave of switching from one stable state  $\theta = \theta_h$  to the other  $\theta = \theta_{\max}$  for the given value of  $\eta = \eta_h$ ,  $\theta = \theta_h$  fully determines the shape and the propagation velocity  $v$  of the wave front—the front wall of the AS. The back wall of the AS is separated from the front wall by the distance  $\mathcal{L}_s \gg l$ . It is followed by the refractory region, in the periphery of which  $\theta$  goes to  $\theta_h$  and  $\eta$  goes to  $\eta_h$ . The velocity of the AS has an upper limit of order  $l/\tau_\theta$ ; and the less is  $\mathcal{L}_s$ , the less is  $v$  [1,2,9,10].

Far from the bifurcation points the amplitude and the velocity of the traveling AS in N systems only weakly depend on the value of  $\alpha \ll 1$  and tend to finite values as  $\alpha \rightarrow 0$ . This allowed us to use standard singular perturbation theory based on the expansion in the powers of the small parameter  $\alpha$ , to construct the solutions in the form of traveling broad AS in N systems [9,10].

At the same time, there is a number of physical [1–3], chemical [12,13], and biological [6,14] systems described by Eqs. (1) and (2) in which the nullcline of Eq. (1) is of V or  $\Lambda$  form. In other words, for these V or  $\Lambda$  systems the equation  $q(\theta, \eta, A) = 0$  has only two solutions,  $\theta_h$  and  $\theta_s$ , for the given  $A$  and  $\eta = \eta_h$ . In this case  $\theta = \theta_s$  corresponds to the region of  $\theta$  and  $\eta$  where  $\partial q / \partial \theta < 0$ , i.e., according to Eq. (1), it corresponds to the unstable state of the system for  $\eta = \text{const}$ . It was found that when  $\epsilon \ll 1$  and  $\alpha \gg 1$ , one can excite static spike AS in such systems. The amplitude of these AS goes to infinity as the small parameter  $\epsilon \rightarrow 0$  [1,2,15].

The existence of traveling wave solutions in  $\Lambda$  and  $V$  systems is one of the fundamental problems of nonlinear physics. However, the standard singular perturbation theory used to construct the solutions in  $N$  systems cannot be applied here. The inapplicability of the standard singular perturbation theory is a general property of  $\Lambda$  and  $V$  systems, in which spike AS form [1,2,15]. As we will show below, for a traveling spike AS it is associated with the fact that, in addition to smooth and sharp distributions (outer and inner solutions) in the traveling spike AS, there exists a region of supersharp distributions, in which the characteristic length of the variation of both the activator and the inhibitor is much smaller than that for the smooth and sharp distributions.

Brusselator—the model of a hypothetical autocatalytic reaction introduced by Nicolis and Prigogine [12]—is a classical model of  $\Lambda$  and  $V$  systems. Equations (1) and (2) for this model are

$$\tau_\theta \frac{\partial \theta}{\partial t} = l^2 \Delta \theta + 1 + \theta^2 \eta - \theta(1 + A), \quad (3)$$

$$\tau_\eta \frac{\partial \eta}{\partial t} = L^2 \Delta \eta - \theta^2 \eta + A\theta. \quad (4)$$

It can be seen that the nullcline of Eq. (3), i.e., the function  $\eta = [\theta(1 + A) - 1]\theta^{-2}$ , is of  $\Lambda$  form, and that the homogeneous state of the system

$$\theta_h = 1, \quad \eta_h = A \quad (5)$$

is stable for  $A < 1$  [2,3].

In the numerical simulations of Eqs. (3) and (4) with  $\alpha \ll 1$ ,  $\epsilon \gg 1$ , and  $A < 1$  in one dimension we found that in some region of the system's parameters there exists a traveling wave solution. Since known spike AS are strongly localized in the regions of size of order  $l$  in which the maximum value of the activator is much greater than  $\theta_h$  [1,2], we expected that traveling spike AS would have a size of order  $l$ , and very large amplitude and velocity. This was taken into account in the numerical simulations. The boundary conditions were neutral. At the initial moment the distribution of  $\eta$  was homogeneous with  $\eta = \eta_h$ , and the distribution of  $\theta$  was taken in the form of a pulse with sufficiently large amplitude and the width of several  $l$  near the right boundary. Outside the pulse  $\theta$  was equal to  $\theta_h$ . Traveling spike AS formed near the right boundary, traveled through the entire space interval, and disappeared at the left boundary.

Figure 1, which represents a solution in the form of the traveling spike AS, shows that the value of the activator in the spike is much greater than 1. Figure 2, in which the AS velocity is plotted versus  $\alpha$  for different values of  $A$ , also shows that, in contrast to the traveling AS in  $N$  systems, where, as was mentioned earlier, the velocity is bounded from above by the value of the order of  $l/\tau_\theta$ , the velocity of the traveling spike AS is much greater than  $l/\tau_\theta$ .

Keeping in mind these facts, let us study the solution in the form of traveling spike AS analytically. We will measure the length and time in units of  $l$  and  $\tau_\theta$ ,

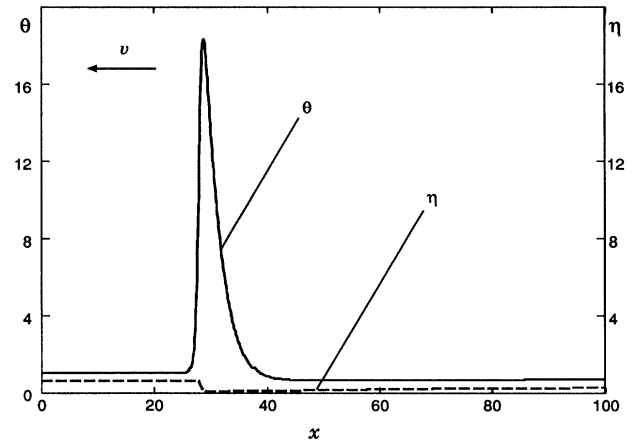


FIG. 1. Distributions of  $\theta(x)$  and  $\eta(x)$  in the form of the traveling spike AS. Numerical solution of Eqs. (3) and (4) for  $\alpha = \tau_\theta/\tau_\eta = 0.02$ ,  $L = 0$ ,  $A = 0.6$ . Autosoliton speed  $v = 2.71l/\tau_\theta$ . Length is measured in units of  $l$ .

respectively. Let us introduce the automodel variable  $z = x + vt$ . Then Eqs. (3) and (4), describing a one-dimensional wave traveling with the velocity  $v$  to the left in the case  $L = 0$ , become

$$v \frac{d\theta}{dz} = \frac{d^2\theta}{dz^2} + 1 + \eta\theta^2 - \theta(1 + A), \quad (6)$$

$$\alpha^{-1} v \frac{d\eta}{dz} = A\theta - \eta\theta^2. \quad (7)$$

Substituting  $\eta\theta^2$  from Eq. (7) into (6) and introducing the new variables

$$\tilde{\theta} = \theta - 1, \quad \tilde{\eta} = \eta - A, \quad (8)$$

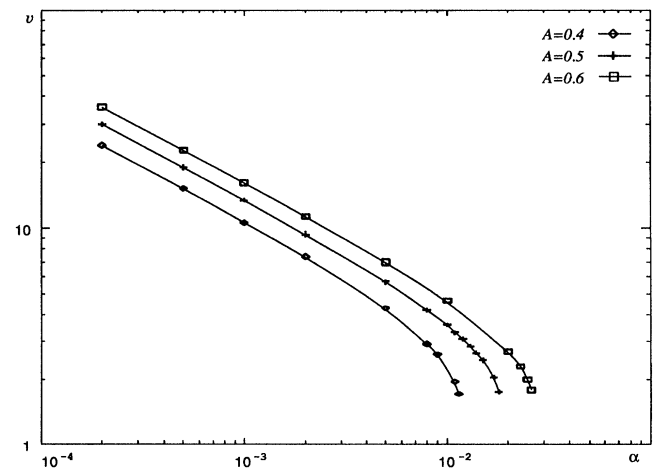


FIG. 2. Dependences of traveling spike AS velocity on  $\alpha$  for different values of  $A$ . Results of the numerical simulations of Eqs. (3) and (4) with  $L = 0$ .

we get the equation

$$\tilde{\theta}_{zz} - v\tilde{\theta}_z - \tilde{\theta} = \alpha^{-1}v\tilde{\eta}_z. \quad (9)$$

Since in our units  $v \gg 1$ , the Green's function of Eq. (9) is approximately

$$G(z, z') = \begin{cases} -\frac{1}{v} e^{v(z-z')}, & z \leq z', \\ -\frac{1}{v} e^{-(z-z')/v}, & z \geq z'. \end{cases} \quad (10)$$

The solution of Eq. (9) with the Green's function from Eq. (10) will then be

$$\tilde{\theta}(z) = -\alpha^{-1} \times \left( e^{vz} \int_z^{+\infty} e^{-vy} \tilde{\eta}'_y dy + e^{-z/v} \int_{-\infty}^z e^{y/v} \tilde{\eta}'_y dy \right), \quad (11)$$

where  $\tilde{\eta}'_y = d\tilde{\eta}(y)/dy$ .

According to the results of the simulations, the distribution of the inhibitor varies sharply only in the region of the AS front wall. After the maximum value of the activator  $\theta_{\max} \gg 1$  is achieved, the inhibitor changes smoothly with the characteristic length  $\alpha^{-1}v$  (Fig. 1). We can distinguish three regions: the region of supersharp distributions where both the activator and the inhibitor vary sharply, the region of sharp distributions where only the activator varies sharply, and the region of smooth distributions where both the activator and the inhibitor vary smoothly. We may assume that the maximum value of  $\theta$  in the spike is reached at  $z = 0$ . Therefore, the region  $z < 0$  will correspond to the supersharp distributions, the region  $z > 0$  will correspond to the sharp distributions, and the region  $z \gg 1$  will correspond to the smooth distributions. In the region of sharp distributions the function  $\eta(z)$  is almost constant. Let us denote this constant as  $\eta_s$ . Since the maximum value of the activator in the spike is much greater than 1,  $\eta_s \ll 1$  in order to satisfy Eq. (7) in the region of sharp distributions. Therefore, in the region of supersharp distributions the inhibitor changes from  $\eta_h = A$  to almost zero. This means that the derivative  $\tilde{\eta}'_z$  in this region is close to a delta function. Let us take

$$\tilde{\eta}'_z = -A\delta(z) \quad (12)$$

and substitute it into Eq. (11). As a result, we get that the solution for the activator in the region of sharp distributions is

$$\theta_{sh}(z) = A\alpha^{-1}e^{-z/v}. \quad (13)$$

Thus, the characteristic length of the activator variation in this region is  $v \gg 1$ , and the maximum value of the activator in the spike is

$$\theta_{\max} = A\alpha^{-1}. \quad (14)$$

Since the characteristic length of the activator's variation in the region of supersharp distributions is much smaller than that in the sharp distribution region, the details of the actual supersharp distribution of  $\eta(z)$  are not important for the sharp distributions. For this reason

Eq. (13) represents the actual sharp distribution of the activator. As in the standard singular perturbation theory, the solution in the region of smooth distributions will be given by Eq. (7) and the equation of local coupling

$$1 + \eta\theta^2 - \theta(1 + A) = 0 \quad (15)$$

obtained from Eq. (6) by equating all derivatives to zero, when  $\eta$  relaxes from  $\eta_s$  to its value  $\eta_h$  in the homogeneous state [1,2]. According to Eqs. (7) and (14),  $\eta_s \approx \alpha$ , i.e., the assumption about the coefficient by the delta function in Eq. (12) is valid with an accuracy  $\alpha$ .

Now let us turn to the supersharp distribution, which determines the velocity of the traveling spike AS. Substituting Eq. (12) into Eq. (11) for  $z < 0$ , we obtain an estimate for the distribution of the activator in the supersharp region:

$$\theta(z) = A\alpha^{-1}e^{vz}. \quad (16)$$

One can see from Eq. (16) that the characteristic length of the activator variation in the region of supersharp distributions is  $v^{-1} \ll 1$ .

Since  $\theta_{\max} \gg 1$  and  $v \gg 1$ , we can approximately rewrite Eqs. (7) and (9) in the region of supersharp distributions, taking into account only their leading terms, as

$$\alpha^{-1}v\tilde{\eta}_z = -(A + \tilde{\eta})\tilde{\theta}^2, \quad (17)$$

$$\tilde{\theta}_{zz} - v\tilde{\theta}_z = \alpha^{-1}v\tilde{\eta}_z. \quad (18)$$

It can be easily seen that the following scaling transformation

$$\begin{aligned} \tilde{\theta}' &= \frac{\alpha\tilde{\theta}}{A}, & \tilde{\eta}' &= \frac{\tilde{\eta}}{A}, \\ v' &= \frac{v\alpha^{1/2}}{A}, & z' &= \frac{zA}{\alpha^{1/2}}, \end{aligned} \quad (19)$$

eliminates the dependence of Eqs. (17) and (18) on  $\alpha$  and  $A$ . This immediately means that the dependence of AS velocity on the system's parameters has the form

$$v = \sqrt{\frac{CA^2}{\alpha}}, \quad (20)$$

where  $C$  is a constant, independent of  $\alpha$  and  $A$ . One can see from Fig. 2 that for sufficiently small  $\alpha$  Eq. (20) holds with very good accuracy with  $C = 0.73$ . One can also see that for  $\alpha$  close to the critical value at which the traveling spike AS disappears, the critical velocity is of order 1, whereas for the traveling wide AS in N systems  $v_c \sim \alpha^{1/2}$  [1,2,10].

Numerical simulations show that the traveling spike AS is stable in a wide range of the system's parameters. When the value of  $A$  is varied, at certain value  $A = A_b$  the traveling spike AS abruptly disappears. At  $A$  close to but greater than  $A_b$ , AS has a velocity of order 1 and amplitude  $\theta_{\max} \gg 1$ . Equation (20) gives an estimate for the value of  $A_b$ . If we take  $v_c \sim 1$ , the value of  $A_b \sim \alpha^{1/2} \ll 1$ .

In the analysis above we ignored the diffusion term in Eq. (4). However, due to its high propagation velocity, traveling spike AS exists in systems with high inhibitor diffusion. Indeed, according to Eq. (14) and the fact that the characteristic length of the activator variation in the supersharp region is of the order of  $\alpha^{1/2}$  [see Eq. (20)], one can see from Eq. (4) that the diffusion term here can be neglected if  $\epsilon \gg \alpha^{1/2}$ . If  $\alpha$  is sufficiently small, this condition can be satisfied by  $\epsilon \ll 1$ , i.e.,  $l \ll L$ . These conclusions are supported by the numerical simulations. For example, for  $\alpha = 0.005$ ,  $A = 0.5$  the minimal value of  $\epsilon$  at which the traveling spike AS exists is  $\epsilon_c = 0.04$ . In this case the critical velocity  $v_c = 2.75$ , that is, of order 1.

Comparing the solution we obtained in the Brusselator model (Fig. 1) with the profiles of the traveling pulses observed in the Belousov-Zhabotinsky reaction [11] and in nerve tissue [7], one can see remarkable similarity between the shapes of the pulses. The pulse is characterized by a steep front, which we associate with the region of supersharp distributions, followed by a region, which we associate with sharp distribution, in which the activator goes down on the considerably greater length scale. Behind the pulse there is a long refractory region that corresponds to the smooth distributions in our picture.

If we add a term  $B\theta^3$  into the right-hand side of Eq. (3), its nullcline will become of N form for  $B = 1$ . This implies that by changing  $B$  from 1 to 0, i.e., by changing only the character of the nonlinearity, one can significantly change the AS type and increase its amplitude and velocity by several orders of magnitude. This effect may play a significant role in understanding the propagation of nerve pulse and the dynamics of chemical waves in Belousov-Zhabotinsky reactions.

In physical systems, such as electron-hole and gas plasmas, the parameter  $A$  is the excitation level. For this reason the conclusion that for  $\alpha \ll 1$  the value

of  $A_b \ll 1$  and  $\theta_{\max} \gg 1$  means that in plasma which is only slightly away from equilibrium one can excite strongly localized regions of high density or temperature of electrons (a kind of fireball) which propagate with high speed in arbitrary directions.

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