

# Persistence of zero velocity fronts in reaction diffusion systems

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Steady, nonpropagating, fronts in reaction diffusion systems usually exist only for special sets of control parameters. When varying one control parameter, the front velocity may become zero only at isolated values (where the Maxwell condition is satisfied, for potential systems). The experimental observation of fronts with a zero velocity over a *finite interval* of parameters, e.g., in catalytic experiments [Barelko *et al.*, Chem. Eng. Sci., **33**, 805 (1978)], therefore, seems paradoxical. We show that the velocity dependence on the control parameter may be such that velocity is very small over a finite interval, and much larger outside. This happens in a class of reaction diffusion systems with two components, with the extra assumptions that (i) the two diffusion coefficients are very different, and that (ii) the slowly diffusing variables has two stable states over a control parameter range. The ratio of the two velocity scales vanishes when the smallest diffusion coefficient goes to zero. A complete study of the effect is carried out in a model of catalytic reaction. © 2000 American Institute of Physics. [S1054-1500(00)01903-0]

**Front propagation plays a crucial role in the dynamics of extended systems. They separate various phases of the systems, and their motion depends on the relative stability of these phases, which depends on some external control parameter. Zero velocity (motionless) fronts are rare solutions in the sense that they typically appear at most once when varying one control parameter. This is what is expected from general considerations in variational systems (notion of Maxwell point). The experimental observation in catalytic reactions of {it intervals} of control parameters where the front velocity is zero is in this context very surprising. In this article we analyze this problem theoretically. Namely, we show that the phenomenon of persistent zero velocity can be understood when the system is described by at least two reaction diffusion equations, with two assumptions about the special form of the equations (existence of two very different diffusion coefficients, and bistability of the slowly diffusive variable over a range of control parameters), compatible with the existing models of catalytic activity over a platinum wire.**

## I. INTRODUCTION

Reaction diffusion waves are observed in a wide range of contexts, including combustion, chemical waves in homogeneous systems, in the presence of a catalytic element, and in a number of biological systems.<sup>1-4</sup> In the case where several equilibrium states coexist, front solutions may describe how a region in the more stable phase grows at the expense

of a less stable state.<sup>5</sup> Control parameters, such as temperature, modify the nature of the equilibrium states. In general, for a special value of the external parameter, the two investigated phases have the same stability. In a thermodynamic context, this occurs at the Maxwell point, where the free energies of the two states are equal. In this situation, the front solutions separating the two states have a zero velocity. This is however a rather special case, corresponding to a restricted set of values of the external parameters (a set of codimension 1).

Mathematically, reaction diffusion systems are governed by partial differential equations of the type

$$\partial_t u = f_\mu(u) + D \partial_x^2 u, \quad (1)$$

where  $\mu$  is the control parameter. When  $u$  is a scalar function, that is, when there is only one reacting species, the front separating the two locally stable states  $u_-$  and  $u_+$  has a zero velocity when the following (Maxwell) condition:

$$\int_{u_-}^{u_+} f_\mu(u) du = 0, \quad (2)$$

is satisfied. Equation (2) is a relation between the control parameters. As a consequence, if one varies only one control parameter, steady front solutions exist only at isolated values of the control parameter, and not on a whole interval.

Even for a reaction diffusion system with an arbitrary number of variables, zero velocity fronts may be observed only for a subset of codimension one of control parameters.<sup>6</sup> This results from very general geometric considerations. Stationary front solutions of reaction diffusion systems with  $n$  components obey the ordinary differential equation

$$\mathbf{D} \partial_x^2 \mathbf{u} + \mathbf{f}_\mu(\mathbf{u}) = \mathbf{0}, \quad (3)$$

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where  $\mathbf{u}=(u_1, \dots, u_n)$  and  $\mathbf{D}$  is an invertible, positive definite matrix. Equation (3) defines a  $2n$ -dimensional dynamical system which is reversible (invariant under  $x \rightarrow -x$ ). Front solutions correspond to heteroclinic trajectories, leaving  $\mathbf{u}_-$  when  $x \rightarrow -\infty$  and approaching  $\mathbf{u}_+$  when  $x \rightarrow +\infty$ . Because of the reversibility, the unstable manifold of  $\mathbf{u}_-$ ,  $\mathcal{W}_u(\mathbf{u}_-)$ , defined as the set of solutions such that  $\mathbf{u} \rightarrow \mathbf{u}_-$  when  $x \rightarrow -\infty$ , and the stable manifold of  $\mathbf{u}_+$ ,  $\mathcal{W}_s(\mathbf{u}_+)$ , the set of solutions such that  $\mathbf{u} \rightarrow \mathbf{u}_+$  when  $x \rightarrow +\infty$ , are both of dimension  $n$ . A heteroclinic trajectory can be found when the two manifolds intersect along a line, (a one-dimensional manifold), in the phase space of dimension  $2n$ .

Geometric arguments show that this does not happen unless an extra condition is imposed on the set of external parameter. As follows from the transversality theory (see, for example, Ref. 7) the dimension of the intersection of two manifolds,  $A$  and  $B$ , in  $N$ -dimensional space is generically

$$\dim(A \cap B) = \dim(A) + \dim(B) - N. \quad (4)$$

In our case,  $N=2n$  and  $\dim \mathcal{W}_u(\mathbf{u}_-) = \dim \mathcal{W}_s(\mathbf{u}_+) = n$ , so the dimension of the intersection of the two manifolds is zero. To make it equal to one, as required for existence of the heteroclinic trajectory, an extra condition should be imposed to the set of control parameters, that forces the dynamics to be restricted to a lower dimension space.<sup>7</sup>

This proves the result stated above: Stationary front solutions of the partial differential Eq. (3) with the proper boundary condition exist only for a subset of external parameters, of codimension one.<sup>6</sup>

In many experiments, zero velocity fronts are observed at one special value of the control parameter, in full agreement with the general considerations above. In contrast, the experimental observation that zero velocity fronts may exist over a whole *interval* of external parameters seems paradoxical. This phenomenon has been observed in waves of catalytic oxidation of ammonium over catalytic wires,<sup>8</sup> as well as in transition from nucleate to film boiling over a heat generating element, a situation that may be described phenomenologically by reaction diffusion systems.<sup>9</sup> An explanation involves the multivalued (hysteretic) character of the function  $f_\mu$  in Eq. (1). The hysteresis is heuristically described with the help of an extra discrete variable, specifying which branch of the function governs the dynamics of the system.<sup>10</sup> In this work, we show that fronts with a *very small velocity* may exist over a finite range of parameters, and with a much larger velocity outside, in a class of coupled reaction diffusion equations for two variables  $u_1$  and  $u_2$  with the following features:  $\mathbf{H}_1$  the two diffusion coefficients are extremely different, say  $D_1 \gg D_2$ , and  $\mathbf{H}_2$  the variable with the small diffusion coefficient has two stable steady states over a range of control parameters.

Because of the hypothesis  $\mathbf{H}_1$ , the width of the region where the variable  $u_2$  changes significantly is very narrow. Assumption  $\mathbf{H}_2$  implies that the reaction term of the variable with the largest diffusion coefficient,  $u_1$ , has several branches, and in this sense, is multivalued. By *very small velocity*, we mean that the velocity is controlled by the smallest diffusion coefficient  $v \sim \sqrt{D_2}$ . This is possible when a

Maxwell condition, Eq. (2) for the variable  $u_1$  is satisfied. When this condition cannot be fulfilled, fronts propagate at a much larger velocity,  $v \sim \sqrt{D_1}$ .

Physically, the fact that the velocity may be very small over a finite range of control parameters, and much larger outside this range provides an explanation for the phenomenon reported in Refs. 8 and 9. In experimental systems, the ratio  $D_2/D_1$  can be as small as  $\sim 10^{-6}$ , therefore, making the small velocity ( $v \sim \sqrt{D_2}$ ) 3 orders of magnitude smaller than the fast velocity ( $v \sim \sqrt{D_1}$ ).

The conditions  $\mathbf{H}_1$  and  $\mathbf{H}_2$  are met in activator-inhibitor systems, with a long range inhibition ( $u_1$  plays the role of the inhibitor, and  $u_2$  of the activator).<sup>11</sup> As such, these assumptions are very plausible in a number of contexts.

We focus here on the problem of chemical reaction over a catalytic element, which we study with the help of an explicit, although somewhat approximate model of catalytic reaction, described in Sec. II.

A number of analytic tools have been developed to investigate excitable systems with long range inhibition. In particular, much effort has been devoted to the appearance of localized structures in these systems (such as the ‘hot spots’,<sup>12</sup> observed in catalytic reaction), see among others.<sup>11,13-16</sup> Using similar analytic techniques, we investigate the existence and the structure of slow fronts in the model of catalytic reaction. The analytic results are confirmed by our numerical study, see Sec. III.

Finally, we investigate the transition from slow to fast waves, when the Maxwell condition cannot be satisfied.

## II. THE MODEL

In this section, we introduce the model to describe catalytic reactions over a platinum wire immersed in a gas stream at temperature  $T_0$ . The dynamics of reactive systems involves, in general, many variable. The model we use has only two variables (the others may be considered adiabatically eliminated):  $T$ , the temperature, and  $n$ , interpreted as ‘active center’ density. This variable, introduced originally by analogy with chain branched reactions, is supposed to reflect structural changes at the surface of the catalyst, as observed very clearly in a number of recent experiments.<sup>17</sup> Other theoretical descriptions of this phenomenon were proposed in Refs. 18 and 19. We will simply use the fact that  $(T, n)$  obey a set of coupled reaction diffusion equations, and that the two diffusion coefficients,  $D_T$  and  $D_n$  (respectively, for temperature and for active centers), have very different orders of magnitude

$$D_n \ll D_T. \quad (5)$$

Physically this comes from the fact that a catalytic wire has a very good thermal conductivity, whereas changes in surface conformation propagate very slowly along the wire.

The model considered explicitly in the present work is

$$\partial_t T = D_T \partial_x^2 T + F(T, n), \quad (6)$$

$$\partial_t n = \frac{D_n}{a} \partial_x^2 n + af(T, n), \quad (7)$$

with

$$F(T, n) = n(1 + \tanh(\gamma(T - T_*))) - \delta(T - T_0), \quad (8)$$

$$f(T, n) = k_1(T)n^2(1 - n) - k_2(T)n + k_3(T). \quad (9)$$

The scaling factor  $a$  is introduced for later purpose. It will be set equal to 1 unless stated otherwise. The first term in the equation for  $F$ , Eq. (8), is the production term. It is proportional to  $n$ , expressing the fact that the reaction can proceed only in the presence of active centers. The assumed temperature dependence is an approximation, which reproduces the main qualitative features of a more realistic dependence: The reaction does not proceed at temperatures appreciably below  $T_*$ , and the reaction rate saturates at high temperature. In the second term, effectively a loss term, the temperature  $T_0$  of the gas stream is taken as our control parameter. The dynamics of active centers is controlled by the reaction term, Eq. (9), which can be justified experimentally.<sup>20</sup> The terms  $k_i(T)$  were effectively shown to be Boltzmann factors:  $k_i(T) = k_i^0(T)\exp(-E_i/RT)$ . We have simplified these factors, and taken  $k_1(T) = \alpha T$ ,  $k_2(T) = 1$  and  $k_3(T) = \beta T$ , which provides a qualitatively correct description of the active center dynamics.

At a given value of  $T$ , the reaction term  $f(T, n)$  is a cubic polynomial in  $n$ , which possesses either three real roots: One stable, typically close to 1, and two close to 0 (one stable and one unstable), or just one stable real root, close to 1 at large temperature, and close to 0 at small temperature, see Fig. 1(a). The disappearance of the branches near  $n \approx 0$  results from the creation term,  $k_3(T)$  in Eq. (9). Because of these features, the front solutions we are looking for may exist only in an interval of temperature. They do not exist above the temperature  $T_u$  where the lower branches of  $n$  disappear, and below  $T_l$  where the higher branch disappears. Figure 1(a) shows that the assumption **H**<sub>2</sub>, stated in the previous section, is satisfied in the model we are considering.

Since the variable  $n$  is essentially bistable over a range of temperature, the function  $F(T, n)$  has two branches, corresponding to each value of  $n$ :  $F_{\pm}(T) \equiv F(T, n_{\pm}(T))$ . One may approximate the upper branch  $F_+(T)$ , for  $T \geq T_l$  and for large enough  $T_0$  and  $\gamma$ , by

$$F_+(T) \approx 2 - \delta \times (T - T_0), \quad (10)$$

and the lower branch  $F_-(T)$  for  $T \leq T_u$  by

$$F_-(T) \approx -\delta \times (T - T_0), \quad (11)$$

see Fig. 1(b). We mention that for sufficiently large  $\gamma$ , models (6)–(9) has three (and even four) stable states coexisting in a limited range of values of  $T_0$ . This leads to unusual regimes of propagation, studied, for example, in Ref. 21. We will not consider these phenomena.

Our analytic study of the reaction diffusion system Eqs. (6)–(9) was complemented by a numerical study. The reaction diffusion system was discretized by using finite differences and integrated in time by a Crank–Nicholson method in a finite domain, with zero flux boundary conditions. In order to look for front solutions, steadily propagating with a finite velocity  $v$ , we replaced in Eqs. (6) and (7)  $\partial_t$  by  $\partial_t - v\partial_x$  (which amounts to use a frame moving at a constant velocity), and adjusted  $v$  so as to reach a steady state. Resolution in this problem is a serious concern, since, as shown

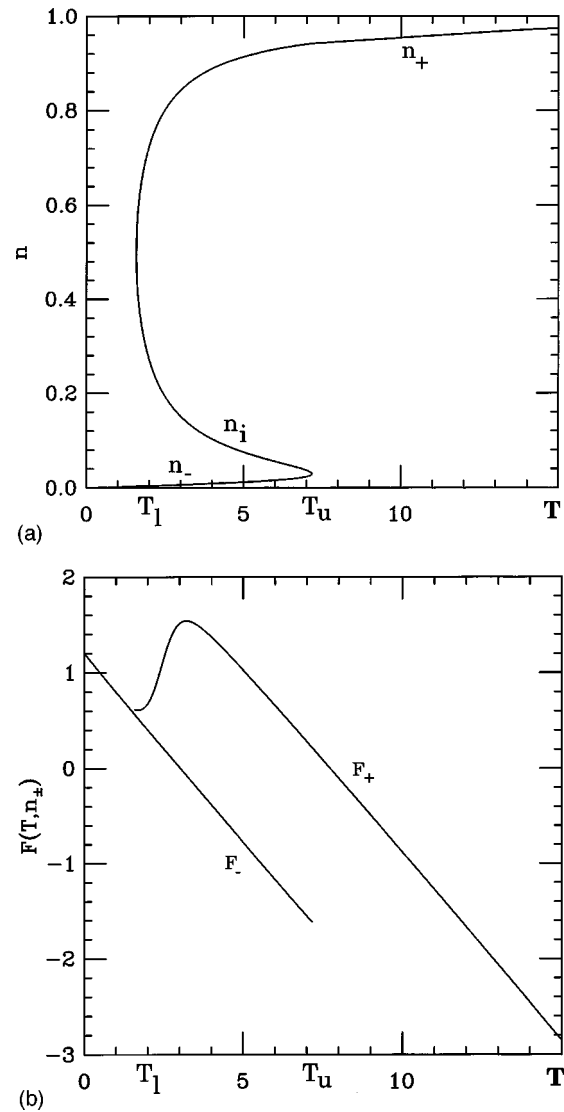


FIG. 1. Bistability in the catalytic model. (a) The roots of  $f(n, T) = 0$  in the  $(T, n)$  plane [Eqs. (6) and (7)]. Three branches of solutions are observed for  $T_l \leq T \leq T_u$ , the highest  $n_+(T)$  and the lowest  $n_-(T)$  are stable. (b) The function  $F_{\pm}(T) \equiv F(T, n_{\pm}(T))$ . As  $T_0$  increases, the two branches move up. The parameters in Eqs. (8) and (9) are  $\alpha = 2.5$ ,  $\beta = 0.002$ ,  $\gamma = 1.8$ ,  $T_* = 2.4$ ,  $\delta = 0.4$ ,  $T_0 = 3$ .

later, the front in  $n$  is very sharp. We insisted that the region where  $n$  varies from  $n \approx 0.2$  and  $n \approx 0.8$  contained at least five grid points. Too low a resolution resulted in unphysical oscillations in the  $n$  profile. We estimate our numerical errors to be at worst of the order of 1%.

### III. SLOW FRONTS

We look for front solutions corresponding to a hot, reactive region ( $n \approx 1$ ), propagating into a colder, inactive region ( $n \approx 0$ ). The mathematical treatment presented in this section is similar to the one used in Ref. 13 to analyze the existence of localized structures in a system with an activator and a long-range inhibitor.

In all cases, when solutions exist, the jump in  $n$  occurs over a very narrow domain, much thinner than the region over which temperature jumps. This is a consequence of Eq.

(5) (our hypothesis  $\mathbf{H}_1$ ). One of the main ideas consists in looking for solutions of the  $n$  equation by simply treating  $T$  as a constant, equal to  $T_j$ . We first consider the case where the polynomial in  $n$ ,  $f(n, T_j)$ , has three roots,  $n_-$ ,  $n_+$  and  $n_i$ , with  $n_+ > n_i > n_-$ ;  $n_+ \approx 1$  and  $n_- \approx 0$ . Steadily propagating front solutions can be readily found by replacing  $\partial_t$  by  $-v \partial_\xi$ ;  $\xi = x - vt$ , in Eq. (7)

$$n(\xi) = \frac{n_+ + n_-}{2} - \frac{n_+ - n_-}{2} \tanh \mu \xi, \tag{12}$$

$$\mu = \frac{n_+ - n_-}{2} \left( \frac{\alpha T_j}{2 D_n} \right)^{1/2}, \tag{13}$$

$$v = \left( \frac{D_n \alpha T_j}{2} \right)^{1/2} (n_+ + n_- - 2n_i)|_{T=T_j}. \tag{14}$$

This solution describes a front propagating at a velocity  $v \sim (D_n \alpha T_j / 2)^{1/2}$ , the variable  $n$  changing from  $n \approx 0$  to  $n \approx 1$  over a distance  $\sim (D_n / T_j)^{1/2}$ . This velocity is proportional to  $\sqrt{D_n}$  and hence quite small.

So far, we have not determined the temperature  $T_j$ , which remains a free parameter in Eqs. (12) and (14). In order to obtain a consistent solution, one has to solve simultaneously the  $T$ -equation, Eq. (7), with the condition that  $n$  jumps from  $n_- \approx 0$  to  $n_+ \approx 1$  at  $T = T_j$ . The equation for  $T$  can be solved by assuming that  $n$  is discontinuous when  $T = T_j$ , which is justified since the region where  $n$  jumps is much narrower than any other distance in the problem. This allows to replace the original equation (7) by

$$-v \partial_\xi T = F_\pm(T) + D_T \partial_\xi^2 T. \tag{15}$$

We consider the case where the velocity is positive, so the system is in the low (respectively high) temperature state when  $\xi \rightarrow +\infty$  (respectively,  $\xi \rightarrow -\infty$ ). Imposing that the location of the front for the  $n$  variable is  $\xi = 0$ , the branch  $F_-$  (respectively,  $F_+$ ) must be chosen for  $\xi \geq 0$  (respectively,  $\xi \leq 0$ ). The problem can be solved analytically when  $F_\pm$  is replaced by its approximate form, Eqs. (10) and (11). By solving in each subdomain, and imposing continuity of the function and its derivative at the boundary, one obtains

$$T(\xi) = T_0 + (T_j - T_0) \exp(\alpha_- \xi) \quad \text{for } \xi \geq 0 \tag{16}$$

and

$$T(\xi) = T_+ + (T_j - T_+) \exp(\alpha_+ \xi) \quad \text{for } \xi \leq 0, \tag{17}$$

where

$$v = \left( \frac{D_T \delta}{2} \right)^{1/2} \frac{(T_+ + T_0 - 2T_j)}{\sqrt{(T_+ - T_j)(T_j - T_0)}}, \tag{18}$$

$$\alpha_\pm \equiv (v/D_T) (-1/2 \pm \sqrt{1/4 + D_T \delta / v^2}),$$

and  $T_+ = T_0 + 2/\delta$ .

In principle, compatibility of Eqs. (14) and (18) fixes the value of  $T_j$ . Since according to Eq. (18), the front velocity is proportional to  $\sqrt{D_T}$ , which is *a priori* much larger than the velocity given by Eq. (14), one obtains  $(T_+ + T_0 - 2T_j) = \mathcal{O}(\sqrt{D_n/D_T})$ . In the limit  $D_n/D_T \rightarrow 0$ , and in the range where Eqs. (10) and (11) apply, one has  $T_j = (T_0 + T_+)/2$ . This coincides with the Maxwell condition

$$\int_{T_0}^{T_+} F(T, n(T)) dT = 0. \tag{19}$$

Quite generally one expects in the limit  $D_n/D_T \rightarrow 0$  the velocity to be given from Eq. (14) with  $T_j$  determined from the Maxwell condition (19) with  $F = F_-$  ( $F = F_+$ ) for  $T < T_j$  ( $T > T_j$ ).

Importantly, because the branches  $n_+$  and  $n_-$  exist only in a finite interval of temperature, the Maxwell construction is possible only in a finite interval of values of  $T_0$ . The disappearance of the  $n_+$  branch at  $T = T_l$  and the  $n_-$  branch at  $T = T_u$  implies that the Maxwell construction, Eq. (19), is possible only if  $T_l \leq T_0 + T_+/2 \leq T_u$ , or equivalently,

$$T_l - 1/\delta \leq T_0 \leq T_u - 1/\delta. \tag{20}$$

In our model the lower limit is only slightly below the zero of the (slow) velocity.

The existence of slowly propagating fronts has been thoroughly checked numerically. An example of such a solution is shown in Fig. 2: Figure 2(a) shows the  $n$ -front, and Fig. 2(b) shows the  $T$ -front. These figures clearly demonstrate the widely different scale of variations for the  $T$  and the  $n$ -profiles.

The dependence of the velocity  $v$  on  $T$  is shown in Fig. 3. It is seen that the slow fronts are observed in an interval of control parameter values where the Maxwell construction is possible. In this range, slow waves are observed: The numerically observed values of the velocity are well described by Eq. (14). The dependence of the velocity on  $\sqrt{D_n}$  has been explicitly checked, see Fig. 3(b).

In the limit  $D_n/D_T \rightarrow 0$ , the temperature  $T_j$  is determined by imposing the Maxwell condition, Eq. (19), and the velocity of the front is small, of order  $\sqrt{D_n}$ . Although the calculation has been carried out completely for a particular model, the conclusion can be generalized for a wide class of functions. This provides a justification of the ideas put forward in order to explain a number of experimental facts,<sup>8,9</sup> and of the work of Petchatnikov and Barelko.<sup>10</sup>

When the condition for existence of slow fronts, Eq. (19), is not satisfied, slow solutions cannot exist.

#### IV. FAST FRONTS

Our numerical results show that steadily propagating front solutions still exist, even when the Maxwell condition Eq. (19) cannot be satisfied. Figure 3 shows that the velocity increases sharply when  $T_0 > T_u - 1/\delta$ , indicating that these fronts have a much larger velocity [see Eqs. (10), (11), and (20)]. The aim of this section is to characterize these fast fronts. We choose to focus here on the disappearance of slow fronts above  $T_0 > T_u - 1/\delta$ . The fast fronts observed on the low-temperature side could be described in a similar way, up to inessential technicalities.

Figure 4 shows an example of front solutions when  $T_0 > T_u - 1/\delta$ . Because of the fact that  $D_n/D_T \ll 1$ , the region where  $n$  jumps is found to be very narrow compared to the length over which  $T$  varies, and therefore the temperature is essentially constant ( $= T_j$ ) in the region of the jump. The structure of fast fronts is in this sense comparable to the structure of slow fronts. However, the gradients observed in

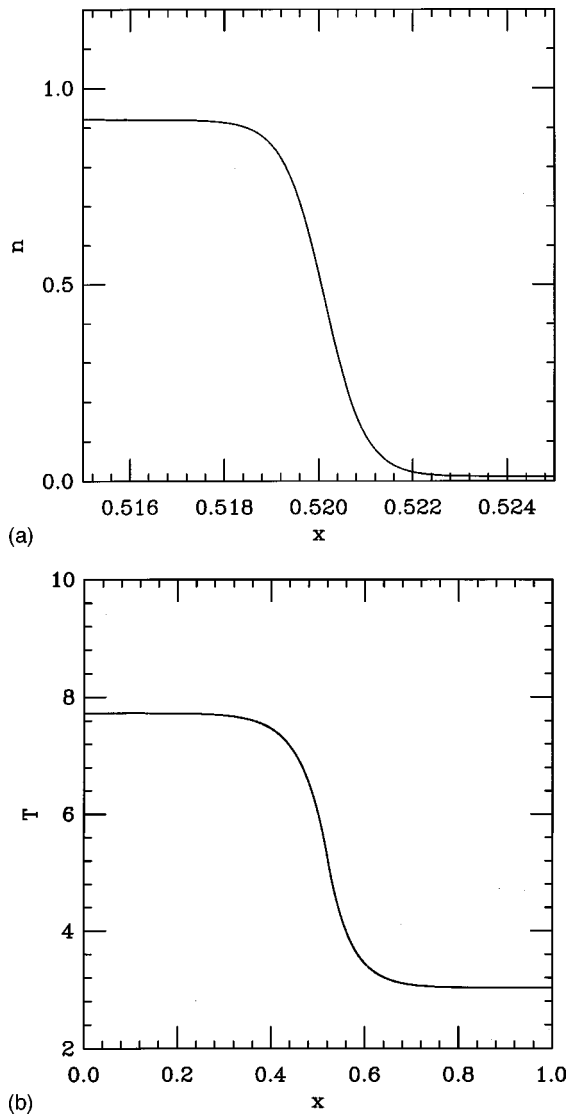


FIG. 2. Structure of a slow front. (a) The  $n$  profile, blown up in the front region. (b) The  $T$  profile, over the entire domain. The  $x$  range in (a) is 100 times smaller than in (b); the temperature is essentially constant in the  $n$  front. The parameters are as in Fig. 1,  $D_n = 10^{-6}$  and  $D_T = 10^{-3}$ .

the fast front case are even larger than the ones observed for slow fronts, compare Figs. 2(a) and 4(a). In addition, one notices a clear lack of symmetry between the upper part and the lower part of the  $n$  front: the value of  $n$  reaches  $n_-$  rather slowly, compared to the sharpness of the front between  $n \approx 0.3$  and  $n = 0.9$ . The contrast between the spatial extent of the foot and the high gradient region increases with  $a$  [see Eq. (7)]. Numerically, the value of  $T_j$  is in the interval  $T_u \leq T_j \leq T_0 + 1/\delta$ .

The fact that the jump in  $n$  may occur at a temperature higher than  $T_u$  seems at first sight paradoxical, since the  $n_-$  branch disappears above  $T_u$ , hence, the solution is expected to jump to the other stable branch,  $n_+ \approx 1$  above  $T_u$ . The explanation for the high values of the temperature  $T_j$  is that although the branches of solutions disappear above  $T_u$ , the function  $f$ , see Eq. (7), remains small near  $n \approx 0$  for  $T \geq T_u$ , hence, the jump in  $n$  does not coincide with the disappearance of the  $n_-$  branch. The temperature  $T_j$  on the

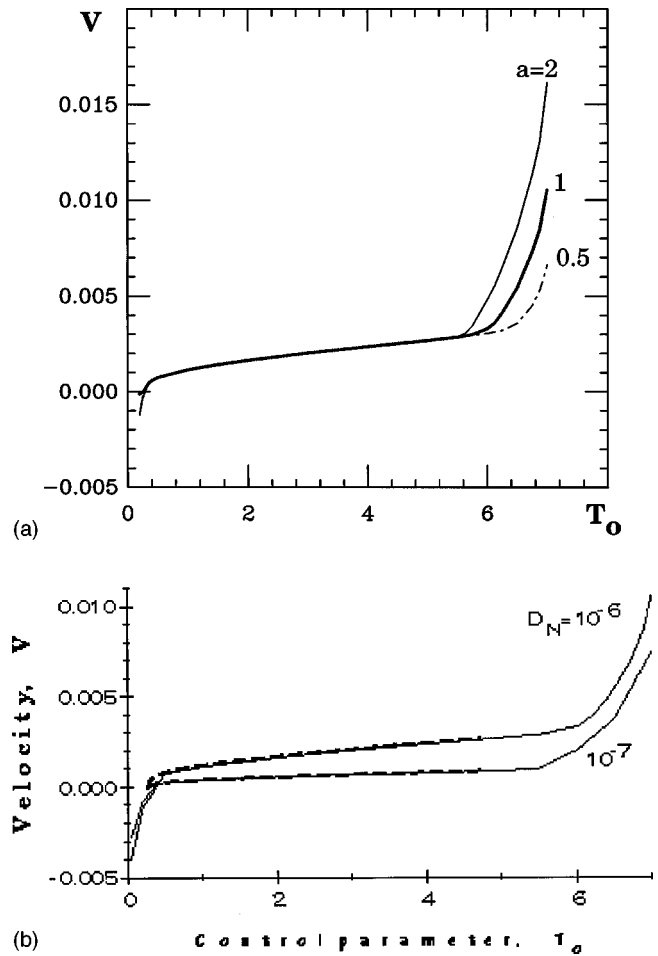


FIG. 3. Velocity of the front as a function of control parameter  $T_0$ . (a) The slow fronts are observed in an interval ( $0.4 < T_0 < 5.6$ ). Parameter  $a$  is introduced in Eq. 7. (b) Influence of the diffusion coefficients. The dashed lines show the fit by Eq. (14). Same parameters as in Figs. 1 and 2. The upper curve corresponds to  $D_n = 10^{-6}$  and  $D_T = 10^{-3}$ , while the lower curve corresponds to  $D_n = 10^{-7}$  and  $D_T = 5 \times 10^{-4}$ .

other hand depends on the strength of the nonlinear term,  $f$ .

To analyze the problem, we make use of the dimensionless parameter  $a$  introduced in Eq. (7) to enhance the nonlinearity. In the temperature range where slow waves exist, the front velocity is independent of  $a$ . However, the width of the front in  $n$  becomes smaller when  $a$  increases, as predicted by Eq. (12) and (13). The situation changes dramatically when slow fronts no longer exist. Figure 3 shows the front velocity for several values of  $a$ , for an otherwise fixed set of parameters. As  $a$  increases the width of the front again becomes smaller, the jump occurs nearer to  $T_u$ , and the front velocity increases. In the limit  $a \rightarrow \infty$  the velocity tends to that obtained from Eq. (18) with  $T_j = T_u$ . It is evident, and we also checked numerically, that the diffusive term in Eq. (7) becomes very small, compared to the other terms in the equation, when  $a$  increases. This suggests that the diffusive term may be dropped when considering large but finite  $a$ .

Since the jump in  $n$  occurs over a very narrow region of space, at a fixed  $T_j$ , the approximate solution Eqs. (16) and (17) for  $T$  should still be valid, as well as the relationship between the velocity  $v$  and  $T_j$ , Eq. (18). Indeed we have checked that Eq. (18) numerically works very well, and that

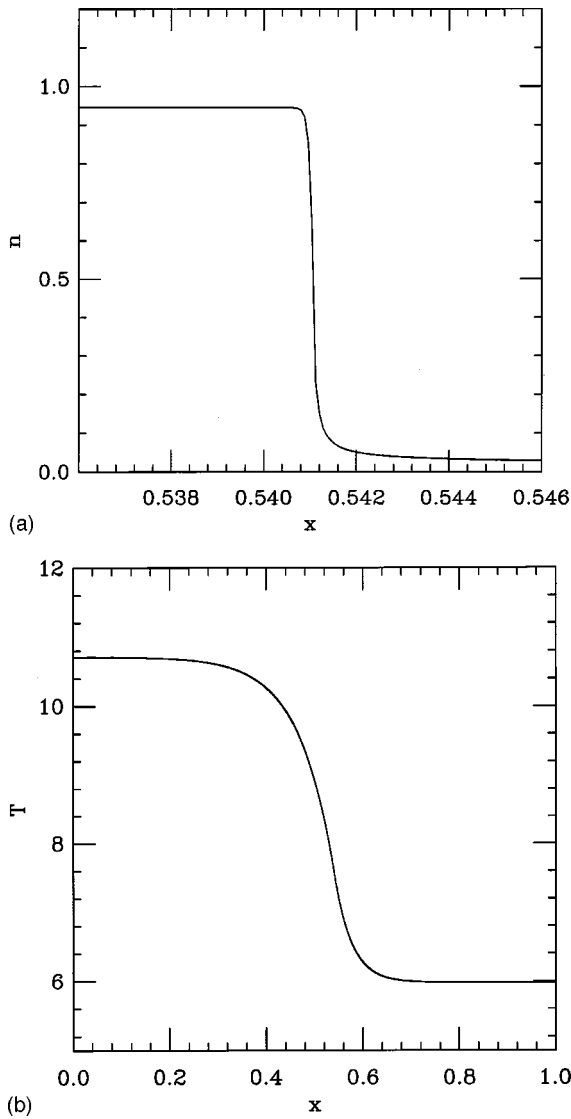


FIG. 4. Structure of a fast front. (a) and (b) are the same as in Fig. 2. A clear lack of symmetry between the upper and the lower parts of the  $n$  front is seen in (a). The parameters are as in Fig. 1,  $T_0 = 5.9$ ,  $a = 32$ ,  $D_T = 10^{-3}$  and  $D_n = 1.6 \times 10^{-5}$ .

the temperature profile is made of two exponentials, as predicted. To completely determine the solution, one has to compute the value of  $T_j$ . Thus the increase of the velocity  $v$  when  $a$  increases is related to the fact that the  $T_j$  to be inserted in Eq. (18) becomes closer to  $T_u$ . The structure of the front may be completely determined in the large  $a$  limit, as we now explain.

The disappearance of the  $n_-$  branch for  $T > T_u$  means that the function  $f$  can be parametrized for  $T \approx T_u$  by

$$f(n, T) = \alpha T_u (n_+ - n) ((n - n_*)^2 + \eta(T - T_u)), \quad (21)$$

where to leading order  $n_+$ ,  $n_*$ , and  $\eta$  are taken at  $T = T_u$ .

In addition, we use the numerically verified fact that the temperature profile is essentially linear between  $T_u$  and the region where the variable  $n$  jumps. The fact that for  $a \rightarrow \infty$  one knows the temperature dependence on  $\xi$  from Eqs. (16) and (17)

$$T(\xi) \approx T_u - \theta \xi, \quad (22)$$

with  $\theta = (T_u - T_0)\alpha_- = (T_u - T_+)\alpha_+$ , leads, after substitution in Eq. (7), and neglecting the diffusion term in the large  $a$  limit, to

$$-v \partial_\xi n = \alpha T_u (n_+ - n) ((n - n_*)^2 - \lambda \xi), \quad (23)$$

where  $\lambda = \theta \eta$ .

In order to solve Eq. (23), we impose as a boundary condition that  $n(\xi)$  is, for large, positive values of  $\xi$ , equal to  $n_-(\xi)$ , the lower branch of solution. With this boundary condition, one may decompose space into (i) a regions where  $n \ll n_+$ , so the equation reduces to the Riccati equation:  $-v dn/d\xi = \alpha T_u n_+ ((n - n_*)^2 - \lambda \xi)$ , and (ii) a region where  $n$  is large.

In region (i), the parameter  $a$  can be scaled away from the Riccati equation

$$-\frac{d\bar{n}}{d\bar{\xi}} = (\bar{n}^2 - \bar{\xi}), \quad (24)$$

by introducing  $n = n_* + e\bar{n}$ ,  $\xi = f\bar{\xi}$ ;  $e = (v/a)^{1/3} (\lambda / \alpha T_u n_+)^{1/3}$  and  $f = (v/a)^{2/3} (1/\alpha T_u n_+)^{2/3} \lambda^{-1/3}$ . The solution of this equation, with the boundary condition  $\bar{n}' = 0$  at  $\bar{\xi} = 0$  has a finite-time singularity,  $\bar{n} \sim 1/(\bar{\xi} - \bar{\xi}_0)$  at  $\bar{\xi}_0 \approx -1.99$ . For other boundary condition the value of  $\bar{\xi}_0$  is changed.

In region (ii) where  $n$  is larger, the  $(n_+ - n)$  term cannot be approximated by a constant any longer. Using the numerical results, we expect that the front is very steep, so  $\xi$  in the right-hand-side (rhs) of the Riccati equation may be replaced by a constant. Scaling distances in the front region by  $\xi = \bar{\xi}(v/a\alpha T_u)$ , one readily finds in the front region

$$-\frac{dn}{d\bar{\xi}} = n^2(n_+ - n), \quad (25)$$

which can be integrated by quadrature. Importantly, the solution of Eq. (25) and the singular solution of Eq. (24) have a common domain of validity, allowing a formal matching.

The result of this analysis is that the front is located at a distance  $\sim (v/a)^{2/3}$  from the location where the  $n_-$  branch disappears. Using again the fact that temperature is linear in the region considered, Eq. (22), and the dependence of  $v$  on  $T_j$ , Eq. (18), our analysis predicts that the front velocity behaves, for large values of  $a$ , as

$$v(a) = v(a = \infty) - \text{const.} a^{-2/3}. \quad (26)$$

In addition, our analysis predicts that the front is very sharp (size of order  $v/a$ ), with a very wide precursor ahead, of size  $(v/a)^{2/3}$ .

This is in full agreement with our numerical results. For a set of parameters, we have varied the parameter  $a$  in the range  $1 \leq a \leq 128$ . The width of the front defined as the difference between the points where  $n = 0.2$  and  $n = 0.8$  is found to scale as  $v/a$ , and the distance between the point where  $T = T_u$  and the location of the jump behaves as  $(v/a)^{2/3}$ . Figure 5 shows the velocity  $v$  as a function of  $a^{-2/3}$ , demonstrating that the numerical results are consistent with the analysis presented above. In fact, the analytic estimate of the prefactor is in fair agreement with the numerical one.

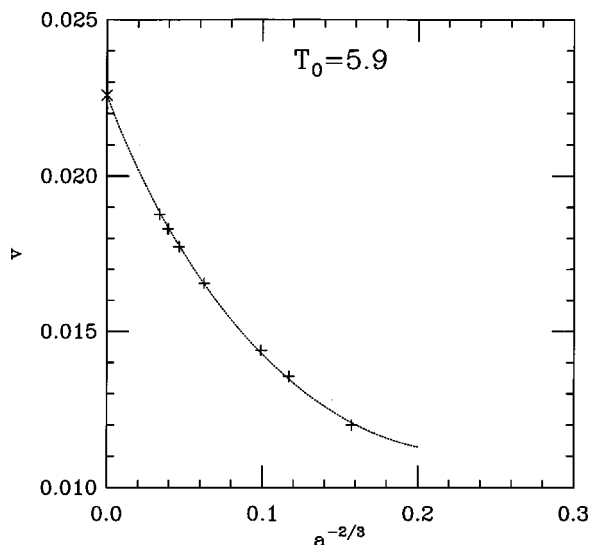


FIG. 5. The velocity of the front as a function of  $a^{-2/3}$ . The numerical values are indicated by + signs, and the limiting value when  $a \rightarrow \infty$  ( $a^{-2/3} = 0$ ) by a cross. The dashed line shows the fitting by a function  $v = v(a = \infty) + A_2 a^{-2/3} + A_3 a^{-1}$ ; with  $A_2 \approx -0.148$  and  $A_3 \approx 0.204$ . In this sense, the numerical results support the analytic prediction, see Eq. (26).

## V. CONCLUSIONS

This work was motivated by the observation of two seemingly contradictory facts. On one hand, the velocity of wave fronts in reaction diffusion systems is zero only for a special subset, of codimension 1, of the set of all the control parameters. This implies that when one parameter is varied, the front velocity should be zero at isolated values, and *not* over a whole interval. On the other hand, in some experimental systems, describable by reaction diffusion systems, the velocity of fronts is found to be zero over some interval of control parameters.

This led us to consider a particular class of reaction diffusion systems, with two variables, and with the two properties  $\mathbf{H}_1$  and  $\mathbf{H}_2$ , spelled out in the introduction. In effect, this problem is very similar to the problem of excitable systems with long range inhibition.<sup>11</sup>

Our work shows that it is possible, under these circumstances, to find a whole interval of parameters over which the front velocity is very small, of order  $\sqrt{D_2}$ . We have shown that the variable  $u_2$  can be effectively eliminated to yield a multivalued function of  $u_1$ . The system chooses, whenever possible, to satisfy a Maxwell condition, Eq. (2). When the Maxwell condition is no longer possible, typically because a branch of solution disappears, faster fronts of velocity  $\propto \sqrt{D_1}$  are observed. The transition between the two regimes has been investigated in our specific model.

Mathematically, the limit  $D_2/D_1 \rightarrow 0$  is a very singular one. From a dynamical system point of view, setting  $D_2 = 0$  amounts to reducing the phase space dimension. In this sense, the limit  $D_2/D_1 \rightarrow 0$  calls for the boundary layer treatment provided here. A better geometric understanding of the problem when  $D_2/D_1 = 0$  is currently being developed.<sup>22</sup>

The conditions  $\mathbf{H}_1$  and  $\mathbf{H}_2$ , necessary to get the conclusions reached in this article, should also apply in other situations, so it should be possible to observe fronts with a very small velocity over some finite range of parameters in other systems as well.

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