Speed of Fronts of the Reaction-Diffusion Equation

R. D. Benguria and M. C. Depassier

Facultad de Física, P. Universidad Católica de Chile, Casilla 306, Santiago 22, Chile

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We study the speed of propagation of fronts for the scalar reaction-diffusion equation \( u_t = u_{xx} + f(u) \) with \( f(0) = f(1) = 0 \). We give a new integral variational principle for the speed of fronts joining the state \( u = 1 \) to \( u = 0 \). No assumptions are made on the reaction term \( f(u) \) other than those needed to guarantee the existence of the front. Therefore our results apply to the classical case \( f > 0 \) in \((0,1)\), to the bistable case, and to cases in which \( f \) has more than one internal zero in \((0,1)\).

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The one dimensional reaction diffusion equation

\[ u_t = u_{xx} + f(u) \quad \text{with} \quad f(0) = f(1) = 0, \quad (1) \]

with \( f(u) \in C^1[0,1] \), has been the subject of much study as it models diverse phenomena in biology, population dynamics, combustion, and others [1–5]. Not only is it in itself of interest, but based on the rigorous results available for this equation diverse methods applicable to pattern forming systems have been developed [6–9]. In applications, the reaction term \( f(u) \) obeys additional requirements depending on the phenomenon being modeled. Three types of nonlinearities appear to be generic, and are shown in Fig. 1. Type A, for which \( f > 0 \) in \((0,1)\) is the classical case of Fisher [10] and Kolmogorov, Petrovskii, and Piskunov (KPP) [11] belongs. Type B, usually referred to as the combustion case, satisfies \( f = 0 \) on \((0,a)\) and \( f > 0 \) on \((a,1)\), while finally, type C, called the bistable case, satisfies \( f(u) < 0 \) for \( u \) in \((0,a)\), \( f > 0 \) on \((a,1)\) with \( \int_a^1 f(u) \, du > 0 \). More general cases for \( f \), namely cases in which \( f \) has more than one internal zero, have also been studied [12,13].

The time evolution of an initial condition \( u(x,0) \) has been studied for all the cases mentioned. It was proved [14] that for suitable initial conditions the disturbance evolves into a monotonic traveling front \( u = q(x - ct) \) joining the stable state \( u = 1 \) to \( u = 0 \). In case A there is a continuum of values of \( c \) for which a monotonic front exists, and the system evolves into the front of minimal speed. In cases B and C there is a single isolated value of the speed for which the front exists. In these last two cases there are threshold effects, and necessary conditions for the evolution of the system into the front have been established as well [12,14]. The same is true for reaction terms with more than one internal zero [12]. The problem which interests us here is the determination of the asymptotic speed of the front. There have been numerous studies of this problem. A very complete review is given in [4]. For reaction terms of type A which in addition satisfy \( f'(0) \geq f(u)/u \) the speed is given by [11] \( c = c_{\text{KPP}} = 2\sqrt{f'(0)} \). For any function of type A this value represents a lower bound on its speed [14]. Another reaction term of type A, that of a function \( f \) approaching a Dirac delta function at \( u = 1 \) was studied in relation to combustion phenomena by Zeldovich and Frank-Kamenetskii. They showed [15] that in that case the speed tends to \( c_{\text{ZFK}} = \sqrt{2} \int_0^1 f(u) \, du \). For an arbitrary reaction function \( f(u) \) a local variational principle of the minimax type exists [4,16]. For reaction terms of types A and B we have shown that an integral variational principle of the Rayleigh-Ritz type exists [17,18]. Recently an interesting conjecture [19] has been put forward for a restricted class of reaction functions.

The purpose of this Letter is to show that the speed of the front joining the state \( u = 1 \) to \( u = 0 \) derives from an integral variational principle without any restriction on \( f \) other than those needed to guarantee the existence of the front. The derivation follows an approach similar to the one used to obtain the principle valid only for positive reaction terms. This new principle, however, which is valid for all cases, is not related, nor equivalent, to the previous one.

![Figure 1](image-url)
It is known [14] that for a function of type A, B, or C there exists a strictly decreasing front \( u = q(x - ct) \) joining \( u = 1 \) to \( u = 0 \) for some \( c > 0 \). The front satisfies \( q_{zz} + cq_z + f(q) = 0 \), \( \lim_{z \to -\infty} u_z = 1 \), \( \lim_{z \to -\infty} u_z = 0 \), where \( z = x - ct \). Following the usual procedure, since the front is monotonic, we define \( p(q) = -dq/dz \), where the minus sign is included so that \( p \) is positive. One finds that the monotonic fronts are solutions of

\[
p(q) \frac{dp}{dq} - cp(q) + f(q) = 0, \tag{2a}
\]

with

\[
p(0) = 0, \quad p(1) = 0, \quad p > 0 \quad \text{in} \quad (0, 1). \tag{2b}
\]

The derivation follows in a simple way from Eq. (2a). Let \( g \) be any positive function in \( (0,1) \) such that \( h = -dg/dq > 0 \). Multiplying Eq. (2a) by \( g(q) \) and integrating between \( q = 0 \) and \( q = 1 \) we obtain, after integration by parts,

\[
\int_0^1 fg \, dq = c \int_0^1 pg \, dq - \int_0^1 \frac{1}{2} hp^2 \, dq. \tag{3}
\]

However, since \( c, p, g, \) and \( h \) are positive, for fixed \( q \), the function

\[
\phi(p) = cpg - \frac{1}{2} hp^2
\]

has a maximum at

\[
p_{\text{max}} = c \frac{g}{h} \tag{4}
\]

so

\[
\phi(p) \leq c^2 \frac{g^2}{2h}
\]

at each value of \( q \). It follows then that

\[
c^2 \geq 2 \frac{\int_0^1 fg \, dq}{\int_0^1 (g^2/h) \, dq}. \tag{5}
\]

This lower bound on the speed is valid for any \( f \) for which a monotonic front exists. To show that this is a variational principle we must show that there exists a function \( g \) at which the equality holds. From Eq. (4) we see that the case of equality is attained when \( \hat{g} \) satisfies the ordinary differential equation

\[
c \frac{\hat{g}}{h} = -c \frac{\hat{g}}{g^\prime} = p .
\]

The maximizing \( \hat{g} \), obtained by integrating this equation, is given by

\[
\hat{g} = \exp \left( -\int_{q_0}^q \frac{c}{p} \, dq \right), \tag{6}
\]

with \( 0 < q_0 < 1 \). Evidently \( \hat{g} \) is positive, monotonic decreasing, and moreover \( \hat{g}(1) = 0 \). Near \( q = 0, \hat{g} \) diverges. We must ensure that the integrals in Eq. (5) exist. To verify this we recall [14] that in the three cases, A, B, and C, the front approaches \( q = 0 \) exponentially. Therefore, near \( q = 0, \)

\[
p \sim \frac{1}{2} \left[ c + \sqrt{c^2 - 4f'(0)} \right] q = mq .
\]

Thus, from Eq. (6) we obtain

\[
\hat{g}(q) \sim \frac{1}{q^{c/m}}
\]

near \( q = 0 \) and \( f \hat{g} \) and \( \hat{g}^2/\hat{g}' \) diverge at most as \( q^{1-c/m} \). Hence, the integrals in Eq. (5) exist if \( m/c > 1/2 \). This condition is always satisfied when \( f'(0) \leq 0 \), that is, in cases B and C. In case A this condition is satisfied provided that \( c > 2\sqrt{f'(0)} \).

Therefore, in cases B and C, and in case A (whenever \( c > c_{\text{KPP}} \)) we have shown that the asymptotic speed of the front is given by

\[
c^2 = \max \left( 2 \frac{\int_0^1 fg \, dq}{\int_0^1 (g^2/h) \, dq} \right), \tag{7}
\]

where the maximum is taken over all positive decreasing functions \( g \) in \( (0,1) \) for which the integrals exist. The maximum is attained when \( g = \hat{g} \).

In case A, if the right side of Eq. (5) does not exceed the linear value \( c^2 = c_{\text{KPP}} = 4f'(0) \) for any \( g \), one can show that the supremum \( \sup \left[ 2 \int_0^1 fg \, dq / \int_0^1 (g^2/h) \, dq \right] \) yields precisely the value \( c^2 = c_{\text{KPP}} = 4f'(0) \). This fact can be seen by choosing the maximizing sequence \( g_a(q) = a(2 - a)u^{a-2} \) with \( 0 < a < 1 \) in the limit \( a \to 0 \).

As an example we may apply the above result to the Nagumo equation which corresponds to a reaction term of the form

\[
f(u) = u(1 - u)(u - a) \quad \text{with} \quad 0 < a < 1/2.
\]

This reaction term is of the bistable type. For this equation the solution to Eq. (2a) is known; it is given by

\[
p(q) = \frac{1}{\sqrt{2}} \sqrt{q(1 - q)}
\]

and the speed is given by

\[
c = \frac{1}{\sqrt{2}} - a\sqrt{2}.
\]

To exhibit in this solvable case that the exact speed can be obtained from the variational principle choose as a trial function

\[
g(q) = \left( \frac{1 - q}{q} \right)^{1-2a}.
\]

The integrals can be performed easily. We obtain

\[
\int_0^1 (-g^2/g') \, dq = \frac{\Gamma(1 + 2a)\Gamma(3 - 2a)}{(1 - 2a)\Gamma(4)}
\]
and
\[ \int_0^1 f g \, dq = \frac{(1 - 2a)(1 + 2a)\Gamma(3 - 2a)}{4\Gamma(4)} \]
so that the lower bound for \( c^2 = (1 - 2a)^2/2 \) which is the exact value. For other nonsolvable cases, it is a simple matter to obtain accurate values for the speed using standard variational techniques.

The calculations performed above for the reaction diffusion equation (1) can be extended in an analogous way to the density dependent diffusion equation
\[ u_t = \frac{\partial}{\partial x} \left[ f(u) \frac{\partial u}{\partial x} \right] + f(u), \quad \text{with } \phi' > 0 \text{ in } (0, 1). \tag{8} \]
For traveling decreasing monotonic fronts \( u = q(x - ct) \) we define \( p(u) = -\phi'(u)u_x \) and proceeding as before we obtain
\[ c^2 \geq 2 \int_0^1 \int_0^1 f \phi' g \, dq \, d\varphi \tag{9} \]
For the density dependent reaction-diffusion equation the existence of monotonic fronts has been established for particular cases of functions \( \phi \) and \( f \) ([20,21] and references therein). For all these cases the bound (9) can be written as a variational principle analogous to (7).

In this Letter we have dealt with a single scalar reaction-diffusion equation. A minimal speed solution is also the relevant asymptotic state for certain classes of systems of reaction-diffusion equations [22–25]. The existence of a variational characterization of the speed in those cases remains to be studied.

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