Chapter 16

VARIATIONAL PRINCIPLES FOR THE SPEED OF TRAVELING FRONTS OF REACTION–DIFFUSION EQUATIONS

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Abstract

The 1D nonlinear diffusion equation has been used to model a variety of phenomena in different fields, e.g. population dynamics, flame propagation, combustion theory, chemical kinetics and many others. After the work of Fisher [Ann. Eugenics 7 (1937) 355] and Kolmogorov et al. [Etude de l'equation de la diffusion avec croissance de la quantité de matiére et son application a un probleme biologique Vol. 1] in the late 1930s, there has been a vast literature on the study of the propagation of localized initial disturbances. The purpose of this review is to present a rather recent variational characterization of the minimal speed of propagation, together with some of its consequences and applications. We consider the 1D reaction–diffusion equation as well as several extensions.

Keywords: reaction diffusion equations; variational principles; combustion; population dynamics; front propagation

Front propagation for the 1D reaction–diffusion equation

$$u_t = u_{xx} + f(u) \qquad \text{with } (x,t) \in \mathbb{R} \times \mathbb{R}_+, \tag{1}$$

with $f(u) \in C^1[0,1]$ and $f(0) = f(1) = 0$, has been the subject of extensive study as it models diverse phenomena in population dynamics [1,2,3], combustion theory, flame propagation [4,5], chemical kinetics and others. There are many important recent reviews on the dynamics of the solutions of the nonlinear reaction–diffusion equation both in the physics literature [6] as well as in the mathematical literature [7,8,9]. We should also point out that the propagation of disturbances in more realistic, and more complicated pattern-forming equations has been the study of many authors, and significant results have been obtained recently (see, e.g. Ref. [10] for the study of the speed of propagation of the Swift–Hohenberg equation, or [11] for the study of the critical speed of traveling waves in the Gross–Pitaevskii equation; see also [12] and many others).

The time evolution for a sufficiently localized initial condition $u(x,0)$ has been studied for different reaction terms. Aronson and Weinberger [13] showed that any positive sufficiently localized (this means decaying faster than exponentially for

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$|x| \to \infty$) initial condition $u(x,0)$ with $u(x,0) \in [0,1]$, evolves into a traveling front propagating at a speed c^* (i.e. for large $t, u(x,t)$ behaves as $q(x - c^* t)$). The shape of the traveling front is determined by the solution to the following two-point boundary-value problem:

$$q'' + cq' + f(q) = 0, \tag{2}$$

with

$$\lim_{x \to -\infty} q(x) = 1 \qquad \text{and} \qquad \lim_{x \to +\infty} q(x) = 0. \tag{3}$$

Aronson and Weinberger characterized the asymptotic speed c^* as the minimum value of the parameter c in Eq. (2) for which the solution $q(x)$ is monotonic. For Fisher's equation, Kolmogorov, Petrovsky and Piskunov (KPP) [2] (see also the translation of this article in Ref. [14]) showed that $c^* = c_{\mathrm{KPP}} = 2$. In fact, for any reaction profile $f(u)$ such that $0 \le f(u) \le f'(0)u$, Kolmogorov et al. proved that $c^* = 2\sqrt{f'(0)}$ (see, e.g. Refs. [2,8,13]). For a general f the speed of traveling fronts for Eq. (1) is unknown in closed form. For this reason, a variational characterization of the speed is an important tool for estimating it. The first variational characterization was obtained by Hadeler and Rothe (see, Ref. [15] and also Theorem 1 in Section 1). The work of Hadeler and Rothe has had many different extensions and applications (see, e.g. the monograph of Volpert et al. [16]). More recently, we have obtained two new different characterizations of the speed of propagation of traveling fronts of Eq. (1), which we will review in the following.

We will distinguish three types of reaction terms.

Case A: $f'(0) > 0, f(u) > 0, u \in (0,1)$. In population dynamics this case is known as *heterozygote intermediate*. This is the case considered in the classical work of Fisher [1] and of Kolmogorov et al. [2].

Case B: There exists $a \in (0,1)$ such that $f(u) \le 0$ for all $u \in (0,a)$, $f(u) > 0$ for all $u \in (a,1)$ and $\int_0^1 f(u)\mathrm{d}u > 0$. This is known as the *combustion case* in the literature.

Case C: There exists $a \in (0,1)$ such that $f(u) < 0$ in $(0,a)$, $f(u) > 0$ in $(a,1)$ and $\int_0^1 \times f(u)\mathrm{d}u > 0$ and $f'(0) < 0$. In population dynamics this case is known as *heterozygote inferior*. It is also known as the *bistable* case.

Our main results, concerning a variational characterization for the speed of propagation of traveling fronts for the nonlinear diffusion equation (1), are contained in the following two theorems. The first variational characterization (Theorem 1) is valid only in Case A, while the second variational characterization (Theorem 2) is valid for all three cases.

Theorem 1 [17]. *Let* $f \in C^1(0,1)$ *with* $f(0) = f(1) = 0, f'(0) > 0$ *and* $f(u) > 0$ *for* $u \in (0,1)$. *Then,*

$$c^* = J \equiv \sup\{I(g) | g \in \mathcal{E}\}, \tag{4}$$

where

$$I(g) = 2\frac{\displaystyle\int_0^1 \sqrt{fgh}\,\mathrm{d}u}{\displaystyle\int_0^1 g\,\mathrm{d}u}, \tag{5}$$

and $\mathcal{E}$ is the space of functions in $C^1(0,1)$ such that $g \geq 0$, $h \equiv -g' > 0$ in $(0,1)$, $g(1) = 0$, and $\int_0^1 g(u)\mathrm{d}u < \infty$. Moreover, if $c^* \neq c_{\mathrm{KPP}} = 2\sqrt{f'(0)}$, J is attained at some $\hat{g} \in \mathcal{E}$, and $\hat{g}$ is unique up to a multiplicative constant.

Theorem 2 [18]. *Let $f \in C^1(0,1)$ with $f(0) = f(1) = 0$, and $\int_0^1 f(u)\mathrm{d}u > 0$. Then,*

$$c^{*2} = L \equiv \sup\{M(g) | g \in \mathcal{F}\}, \tag{6}$$

where

$$M(g) = 2\frac{\int_0^1 fg\mathrm{d}u}{\int_0^1 (g^2/h)\mathrm{d}u}, \tag{7}$$

and $\mathcal{F}$ is the space of functions in $C^1(0,1)$ such that $g \geq 0$, $h \equiv -g' > 0$ in $(0,1)$, $g(1) = 0$, and the integrals in Eq. (7) exist. Moreover, if f belongs to cases B or C, or to Case A with $c^* \neq c_{\mathrm{KPP}} = 2\sqrt{f'(0)}$, L is attained at some $\hat{g} \in \mathcal{F}$, and $\hat{g}$ is unique up to a multiplicative constant.

These two theorems have been extended in several directions. In this review, we give the complete proof of these two variational characterizations (see Section 1), we provide the analogous results for the case of density-dependent reaction–diffusion equations (see Section 2). In Section 3, we apply these theorems to obtain some properties of thermal combustion waves. Finally, in Section 4, we obtain a variational characterization for the minimal speed of fronts for the reaction–convection–diffusion equation.

1. Variational principles for the speed of propagation of traveling fronts

For a general profile $f(u)$, the speed of propagation of traveling fronts for Eq. (1) is not known in closed form. However, there are several variational characterizations of the speed of propagation of the fronts that offer the possibility of accurately estimating it. The first variational characterization was derived by Hadeler and Rothe [15]. They considered the general continuously differentiable nonlinearity $f(u)$, satisfying,

$$f(0) = f(1) = 0,\ f(u) > 0,\ \text{for } u \in (0,1),\ f'(0) > 0,\ f'(1) < 0. \tag{8}$$

Their variational characterization is embodied in the following min–max theorem.

Theorem 1.1 (Hadeler and Rothe, [15], Theorem 8, pp. 257). *The speed of propagation of the traveling fronts of Eq. (1) is given by*

$$c^* = \inf_{\rho} \sup_{u\in(0,1)} \left[\rho'(u) + \frac{f(u)}{\rho(u)} \right], \tag{9}$$

where ρ *is any continuously differentiable function on* $[0, 1]$ *such that*

$$\rho(u) > 0,\ u \in (0,1),\ \rho(0) = 0,\ \rho'(0) > 0. \tag{10}$$

Remark 1.2 For extensions of the variational characterization of Hadeler and Rothe as well as many applications see the monograph [16].

Before we go into the details of the proof of Theorems 1 and 2 a heuristic argument concerning the solutions of Eq. (2) is in order. In all three cases Eq. (2) can be viewed as Newton's equation for a particle moving in one dimension under the action of the force $-f(q) - cq'$ (the variable x now plays the role of time). The force $-f(q)$ is conservative and derives from a potential $V(q) = \int_0^q f(s)\mathrm{d}s$. If $f(q)$ belongs to Case A, the potential is monotonic in (0,1), it has its minimum at the point $q = 0$, and maximum at $q = 1$. The second term, i.e. $-cq'$ represents a viscous force, and, with this picture in mind the parameter c represents the *viscosity* or viscous coefficient. In summary, Eq. (2) is Newton's equation for a particle coming down from the top of the potential at $q = 1$ to the bottom of it at $q = 0$ in the presence of a viscous force. If the *viscosity* (i.e. the parameter c, which is precisely our object of interest here) is small the particle will oscillate near the bottom of the well before it settles down at the minimum (i.e. at $q = 0$). If we increase the *viscosity*, we will reach a value for which there will no longer be oscillations. That is, the particle will come down monotonically from $q = 1$ to $q = 0$ (in mechanics this is commonly known as *critical damping*). It is intuitively clear that if one increases the *viscosity* even further, the particle will also go down monotonically. So, there is a critical value of c, which we denote by c^*, such that for $c \geq c^*$, there will be monotonic decreasing solutions of Eqs. (2) and (3). This fact was proven rigorously by Aronson and Weinberger, and more importantly, they showed that this critical value c^* will be the speed of propagation of fronts of the reaction–diffusion equation (1) (for a sufficiently localized initial condition). If $f(u)$ belongs to Case C, the potential has two maxima, at $q = 0$ and $q = 1$, and a minimum at $q = a$. In this case, the particle starts at $q = 1$ at *time* $x = -\infty$ and it should get to $q = 0$ at $x = \infty$ with zero speed. Because of *energy dissipation*, for this motion to be possible, the maximum at $q = 0$ must be smaller than the maximum at $q = 1$ (otherwise the particle would never reach $q = 0$). In terms of the force f, this condition in the potential implies $\int_0^1 f(q)\mathrm{d}q > 0$. Now, it should be intuitively clear that there is only one value of the *viscosity* c for which the particle will go from the maximum of the potential at $q = 1$ to the valley at $q = a$ and then up to the maximum of the potential at $q = 0$. This is precisely the value c^*. If c is larger than c^* the particle will be trapped forever at the valley. On the other hand, if $c < c^*$ the particle will overshoot at $q = 1$. All these facts have been proven in Ref. [13].

Following the results of Aronson and Weinberger, we are interested in computing the minimal speed for which Eq. (1) has a monotonic traveling front $u(x, t) = q(x - ct)$ joining

$u = 1$ to $u = 0$. The shape of the traveling front will be determined by the monotonic solution of Eqs. (2) and (3). Since q is monotone, in order to analyze the solution to Eqs. (2) and (3), it is convenient to work in phase space. Calling $z = x - ct$, the argument of q, and $p(q) = -\mathrm{d}q/\mathrm{d}z$ (here, the minus sign is included so that p is non-negative), we find that in phase space the monotonic fronts are the non-negative solutions of the following two-point boundary-value problem,

$$p\frac{\mathrm{d}p}{\mathrm{d}q} - cp(q) + f(q) = 0, \qquad \text{in } (0,1), \tag{11}$$

and

$$p(0) = p(1) = 0. \tag{12}$$

In Ref. [13], Section 4, Aronson and Weinberger proved that there is a unique non-negative solution p to Eqs. (11) and (12) for $c = c^*$. Moreover, the solution p is such that $p(q) \approx |m|q$ near $q = 0$, where $|m|$ is the largest root of the equation

$$x^2 - c^* x + f'(0) = 0, \tag{13}$$

i.e.

$$|m| = \frac{1}{2}\left(c^* + \sqrt{c^{*2} - 4f'(0)}\right).$$

It is convenient to introduce the parameter σ as $\sigma = c^*/|m|$. In terms of σ one can write

$$c^* = \sigma\sqrt{f'(0)/(\sigma - 1)} \qquad \text{and} \qquad |m| = \sqrt{f'(0)/(\sigma - 1)}. \tag{14}$$

It is straightforward to verify that whenever $1 < \sigma < 2$ the value of $|m|$ given by Eq. (14) corresponds to the largest root of Eq. (13) and therefore to the asymptotic slope at the origin of the selected front [19]. If $\sigma = 2$ then c^* is given by the *linear* value $c_{\mathrm{KPP}} = 2\sqrt{f'(0)}$.

Proof of Theorem 1 The proof of the theorem is done in two steps. First, we show that

$$c^* \geq J, \tag{15}$$

and then we show that equality actually holds in Eq. (15). To prove Eq. (15) it is enough to show that $c^* \geq I(g)$ for all $g \in \mathcal{E}$. Multiply Eq. (11) by g/p, for any fixed $g \in \mathcal{E}$, and integrate over $q \in [0, 1]$. After integration by parts we have,

$$c^* = \frac{\int_0^1 (hp + (fg)/p)\,\mathrm{d}q}{\int_0^1 g\,\mathrm{d}q} \geq I(g), \tag{16}$$

which follows from the fact that

$$hp + \frac{fg}{p} \geq 2\sqrt{fgh},$$

since p, h, f, and g are positive for $q \in (0, 1)$. To finish the proof we have to show that the equality holds in Eq. (15). From the results of Ref. [13] it follows that $c^* \geq 2\sqrt{f'(0)}$. We separate the proof that equality holds in Eq. (15) into two cases: Case (i) $c^* = 2\sqrt{f'(0)}$, and Case (ii) $c^* > 2\sqrt{f'(0)}$. In Case (i), consider the family of functions $g_\alpha(u) = u^{\alpha-1} - 1$, with $0 < \alpha < 1$. Then, $g_\alpha \in \mathcal{E}$ and $\lim_{\alpha \to 0} I(g_\alpha) = 2\sqrt{f'(0)}$ (see, e.g. the appendix of Ref. [20] for a detailed proof of this fact). Hence, from Eq. (15) we have

$$c^* \geq J \geq 2\sqrt{f'(0)},$$

which implies $J = c^*$ in this case.

In Case (ii), we will not only prove that the equality in Eq. (15) holds but also that there exists $\hat{g} \in \mathcal{E}$ with $c^* = I(\hat{g})$. Let $p(q)$ be the positive solution of Eq. (11) satisfying Eq. (12). The existence of such a solution has been established in Ref. [13]. Moreover, $p(q) \approx |m|q$ near $q = 0$. A function $\hat{g}$ will saturate the bound Eq. (16) if and only if,

$$hp = \frac{f\hat{g}}{p}, \tag{17}$$

where $h = -\hat{g}'$ and p is the solution of Eq. (11) mentioned above. Eq. (17) is a first-order ordinary differential equation for $\hat{g}$, whose solution can be written in terms of p as

$$\hat{g}(q) = \frac{p(q)}{c^*} \exp\left(\int_q^{q_0} \frac{c^*}{p} \mathrm{d}q\right), \tag{18}$$

for some fixed $0 < q_0 < 1$. To complete the argument we only need to show that $\hat{g} \in \mathcal{E}$. It follows from Eqs. (17) and (18) that

$$\hat{h}(q) = \frac{g(q)}{c^* p(q)} \exp\left(\int_q^{q_0} \frac{c^*}{p} \mathrm{d}q\right)$$

in (0,1). Moreover, since $p(q) > 0$ in (0,1) and $p \in C^1(0, 1)$ we have that $\hat{g} \in C^1(0, 1)$. Thus, $\hat{g}$ is a continuous, positive and decreasing function in (0,1). Hence, $\hat{g}$ is bounded away from the origin. In order to show that $\int_0^1 \hat{g}(q)\mathrm{d}q$ is finite we have to determine the behavior of $\hat{g}$ near $q = 0$. Since $p \approx |m|q$ near 0, we have from Eq. (18) that

$$\hat{g}(q) \approx \frac{1}{\sigma} \frac{1}{q^{\sigma-1}}$$

near zero. Therefore, if $\sigma < 2$ (i.e. if $c^* > c_{\mathrm{KPP}} = 2\sqrt{f'(0)}$, we have $\int_0^1 \hat{g}(q)\mathrm{d}q < \infty$ and $\hat{g} \in \mathcal{E}$. □

Proof of Theorem 2 Now take $g \in \mathcal{F}$. Multiplying Eq. (11) by $g(q)$ and integrating over $q \in [0, 1]$, we have, after integration by parts, the equality

$$\int_0^1 fg\mathrm{d}q = c\int_0^1 pg\mathrm{d}q - \frac{1}{2}\int_0^1 hp^2\mathrm{d}q. \tag{19}$$

For positive c, g, and h, the function $\varphi(p) = cpg - hp^2/2$ has its maximum at $p = cg/h$, and so $\varphi(p) \leq c^2g^2/(2h)$. It follows that $c^2 \geq M(g)$, which implies (setting $c = c^*$ if c is nonunique) that c^{*2} is no less than the supremum of Eq. (6). Next we show that the equality holds for a function $\hat{g}$. Notice that the condition $p = cg/h$ is solvable in g and gives the expression for the maximizer $\hat{g}$,

$$\hat{g} = \exp\left(-\int_{q_0}^{q} \frac{c}{p}\mathrm{d}q\right), \tag{20}$$

with $q_0 \in (0,1)$. Clearly, $\hat{g}$ is positive and decreasing, with $\hat{g}(1) = 0$ since $p \approx O(1-q)$ for $q \approx 1$. At $q = 0$, however, $\hat{g}$ diverges since the exponent goes to $+\infty$. We must ensure that the integrals on the right side of Eq. (7) exist. To verify this we recall that in the three cases, A, B and C, the front approaches $q = 0$ exponentially [13]. Therefore, near $q = 0$,

$$p \approx \frac{1}{2}\left(c + \sqrt{c^2 - 4f'(0)}\right)q \equiv mq.$$

Thus, from Eq. (10) we obtain $\hat{g}(q) \approx q^{-c/m}$, near $q = 0$. Hence, both $f\hat{g}$ and $\hat{g}^2/h$ diverge at most as $q^{1-c/m}$ near $q = 0$. Therefore, the integrals on the right side of Eq. (7) exist if $m/c > 1/2$. This condition is always satisfied when $f'(0) \leq 0$, i.e. in Cases B and C. In Case A this condition is satisfied provided $c > c_{\mathrm{KPP}} = 2\sqrt{f'(0)}$. This concludes the proof in Cases B, C, and also in Case A for $c \neq c_{\mathrm{KPP}}$. Finally, in Case A, if $c^* = c_{\mathrm{KPP}}$ one can take the maximizing sequence $g_\alpha = q^{\alpha-2} - 1$, which is in $\mathcal{F}$ for $0 < \alpha < 1$, and let $\alpha \to 0$. One can verify that $\lim_{\alpha\to 0} M(g_\alpha) = 4f'(0) = c_{\mathrm{KPP}}^2$, and we are done. □

2. Variational principle for the asymptotic speed of fronts of the density-dependent reaction–diffusion equation

Several problems arising in population growth [21,22], combustion theory (see, e.g. Ref. [23] and references therein), chemical kinetics [24] can be modeled by an equation of the form

$$\frac{\partial u}{\partial t} + \vec{\nabla}\cdot\vec{j} = f(u),$$

where the source term $f(u)$ (which depends on the density u) represents net growth and saturation processes. In general, the flux $\vec{j}$ is given by Fick's law

$$\vec{j} = -D(u)\vec{\nabla}u,$$

where the diffusion coefficient $D(u)$ in general may depend on the density u. In one dimension this leads to the equation

$$u_t = (D(u)u_x)_x + f(u). \tag{21}$$

We will assume that the reaction term $f(u) \in C^1[0,1]$ satisfies

$$f(u) > 0, \text{ in } (0,1) \text{ and } f(0) = f(1) = 0, \tag{22}$$

(i.e. f is of type A), restrictions that are satisfied by several models. We will first consider here the case when the diffusion coefficient follows a power law (i.e. $D(u) = mu^{m-1}$, for $m \geq 1$). Thus, the equation we consider here is

$$u_t = (u^m)_{xx} + f(u), \tag{23}$$

with f satisfying Eq. (22). Aronson [21], and Aronson and Weinberger [13] have shown that the asymptotic speed of propagation of sufficiently localized initial disturbances for Eq. (23) is the minimal speed $c^*(m)$ for which there exists a monotonic traveling front $u(x,t) = q(x - ct)$ joining $q = 1$ to $q = 0$. The equation satisfied by q is,

$$(q^m)_{zz} + cq_z + f(q) = 0, \tag{24}$$

with

$$q(-\infty) = 1, q > 0,\ q' < 0 \text{ in } (-\infty, \omega) q = 0 \ \text{ for } \ z \geq \omega, \tag{25}$$

where $z = x - ct$. When $m > 1$ the wave of minimal speed is *sharp*, i.e. $\omega < \infty$ [21].

We can also give a variational characterization of the speed $c^*(m)$ for the density-dependent reaction–diffusion equation. This is given by the following theorem.

Theorem 2.1 [19,25]. *If f is of type A, then,*

$$c^*(m) = \max\left(\frac{2\int_0^1 \sqrt{mq^{m-1} fgh}\,\mathrm{d}q}{\int_0^1 g\,\mathrm{d}q} \right), \tag{26}$$

where the maximum is taken over all functions g for which the integrals in Eq. (26) exist and $g(0) = 1, g(1) = 0$, and $h = -g' > 0$. Moreover, there is a unique g for which the maximum is attained.

Proof: We follow the same method as in the proof of Theorem 1. We go to phase space, but this time we denote $p(q) = -q^{m-1}\mathrm{d}q/\mathrm{d}z > 0$, which is positive since the selected speed corresponds to that of a decreasing monotonic front. Then, $p(q)$ satisfies

$$p\frac{\mathrm{d}p}{\mathrm{d}q} - \frac{c^*}{m}p + \frac{1}{m}q^{m-1}f(q) = 0, \tag{27}$$

with

$$p(0) = p(1) = 0, p > 0 \text{ in } (0,1). \tag{28}$$

Although the wave of minimal speed is *sharp* and therefore $q'(0) < 0$, by the definition of p, we still have $p(0) = 0$. Multiplying Eq. (27) by a function g (such that $g(0) = 1$, $g(1) = 0$, and $h = -g' > 0$), integrating over $q \in (0,1)$, using integration by parts and the Schwarz inequality as in the proof of Theorem 1 above, we get

$$c^*(m) \geq \left(\frac{2\int_0^1 \sqrt{mq^{m-1} fgh}\,\mathrm{d}q}{\int_0^1 g\,\mathrm{d}q} \right). \tag{29}$$

To finish the proof, we need only show that there is a function g for which equality is obtained in Eq. (29). Equality is obtained in Eq. (29) if

$$\frac{1}{m}q^{m-1}f(q)\frac{g}{p} = ph = -pg'(q), \tag{30}$$

which is an ordinary differential equation for g, in terms of p, whose solution can be written as

$$g(q) = \frac{mp(q)}{c^*}\exp\left(-\int_{q_0}^{q}\frac{c^*}{mp(q')}\mathrm{d}q'\right), \tag{31}$$

where $0 < q_0 < 1$. Since $p(1) = 0$ and p is positive in (0,1) it follows that $g(1) = 0$. On the other hand, the function g is bounded at $q = 0$ as we now show. Call $\hat{c} = c^*/m$ and $F(q) = q^{m-1}f(q)/m$. Then Eq. (27) reads

$$pp' - \hat{c}p + F = 0, \tag{32}$$

with $F(0) = F(1) = 0$ and $F'(0) = 0$. For this case Aronson and Weinberger [13] have shown that $p(q)$ approaches $q = 0$ as $p = \hat{c}q = c^*q/m$. Hence, from the differential equation satisfied by g one can show that g approaches a constant as $q \to 0$. We can always normalize this constant to be one by an appropriate scaling of g. Therefore, $g \in C^1([0, 1])$ and the integrals on the right side of Eq. (26) exist for g given by Eq. (31). □

As in the case of the nonlinear reaction–diffusion Eq. (1), there is also a second variational principle in this case. It is given by the following theorem, whose proof is similar to the proof of Theorem 0.2 above, and we leave it to the reader.

Theorem 2.2 *If f is of type A, then,*

$$c^*(m)^2 = 2m \max_{g}\left(\frac{\int_0^1 gf(q)q^{m-1}\mathrm{d}q}{\int_0^1 (g^2/h)\mathrm{d}q}\right), \tag{33}$$

where the maximum is taken over all functions g for which the integrals in Eq. (33) exist and $g(1) = 0$, and $h = -g' > 0$. Moreover, there is a unique g (up to a multiplicative constant) for which the maximum is attained.

As an application consider the case $f(q) = q(1-q)$ and $m = 2$ for which the exact solution is known. Using the variational characterization (Eq. (33)), with the trial function $g(q) = (1-q)/q$, we find

$$c^{*2} \geq 4\frac{\int_0^1 q(1-q)^2\mathrm{d}q}{\int_0^1 (1-q)^2\mathrm{d}q} = 1,$$

the exact value, which is just a reflection of the fact that the maximum is attained precisely at this particular g. In addition, due to the existence of the variational principle we may use the Feynman–Hellmann formula to determine the dependence of $c^*(m)$ on m or, on the possible parameters of a general reaction term f. We illustrate this by applying it to the calculation of $\mathrm{d}(c^*)^2/\mathrm{d}m$ at $m = 2$ (i.e. around the exactly solvable case). By the Feynman–Hellmann theorem, we have from Eq. (33),

$$\frac{\mathrm{d}(c^*)^2}{\mathrm{d}m} = 2\frac{\int_0^1 \hat{g}f(q)[q^{m-1} + m(m-1)q^{m-1}\log q]\mathrm{d}q}{\int_0^1 (\hat{g}^2/\hat{h})\mathrm{d}q}, \tag{34}$$

where $\hat{g}$ is the maximizer in Eq. (33). In the case $f(q) = q(1 - q)$ and $m = 2$, the actual maximizer is $\hat{g} = (1 - q)/q$, so from Eq. (34) we get

$$\left.\frac{\mathrm{d}(c^*)^2}{\mathrm{d}m}\right|_{m=2} = 6\int_0^1 (1-q)^2 q(1 + 2\log q)\mathrm{d}q = -\frac{7}{12}, \tag{35}$$

the value previously obtained by other methods [26,27] (see also Ref. [25] for an alternative derivation using instead the first variational characterization (Theorem 2.1) and the Feynman–Hellmann theorem).

Recently, Malaguti and Marcelli [28] have studied the effects of a degenerate diffusion term in reaction–diffusion models. They study the equation,

$$u_t = (D(u)u_x)_x + f(u), \qquad \text{in } \mathbb{R}^+ \times \mathbb{R}, \tag{36}$$

where both f and D are in $C^1[0,1]$. Their main result is the following theorem.

Theorem 2.3 [28] *Consider Eq. (36) with D and f in* $C^1([0,1])$, *and the reaction term, f, is of type A, while D satisfies,* $D(0) = 0, D'(0) > 0$ *and* $D(u) > 0$ *for all* $u \in [0,1]$. *Then, there exists a constant* c^* *such that Eq. (36) has*

(a) *no traveling wave solutions for* $0 < c < c^*$;
(b) *a monotone traveling wave solution of sharp type with wave speed* c^*.
(c) *a monotone traveling wave, q, of front type, with* $q(-\infty) = 1$ *and* $q(+\infty) = 0$, *for every wave speed* $c > c^*$.

Moreover, it holds that

$$0 < c^* \leq \sqrt{\sup_{q\in(0,1]} \frac{D(q)f(q)}{q}}. \tag{37}$$

Finally, for all $c \geq c^*$ *the wave front, respectively of front or sharp-type, is unique up to translations.*

As before, we can characterize the value of c^* of Theorem 2.3 by the following variational principle.

Theorem 2.4 *Let D and f as in Theorem 2.3, then,*

$$c^* = 2\sup_g \left(\frac{\int_0^1 \sqrt{fgh}\,\mathrm{d}q}{\int_0^1 g\,\mathrm{d}q} \right), \tag{38}$$

where $h \equiv -D(u)g'(u)$, *and the sup is taken on the set of functions* g, *such that* $g \in C^1([0,1])$, $g > 0$ *in* $(0,1)$, $g(1) = 0$, *and* $h > 0$ *in* $(0,1)$.

Remarks 2.5 (i) the proof of this theorem is analogous to the proof of Theorems 1 and 2.1 above and we omit it here. (ii) Using the convexity of the mapping, $t \rightarrow \sqrt{t}$, Jensen's inequality, and integration by parts we can obtain the bound (Eq. (37)) directly from our variational principle (Eq. (38)).

3. Variational calculations for thermal combustion waves

In the simplest model of thermal propagation of flames one is led to the 1D reaction–diffusion Eq. (1), where typically the reaction term is given by the Arrhenius law, which in a reduced version is given by

$$f(u) = (1-u)^r [\mathrm{e}^{\beta(u-1)} - \mathrm{e}^{-\beta}], \tag{39}$$

(see, e.g. Refs. [5,23]) where the term $\exp(-\beta)$ is introduced to remedy the cold-boundary problem [4,29]. The degree of localization of the reaction zone is measured by the Zeldovich number β. For large values of β, the width of the reaction zone is narrow and the speed of propagation of the flame is given by the Zeldovich–Frank–Kamenetskii (ZFK) formula [5],

$$c_{\mathrm{ZFK}} = \left(2\int_0^1 f(u)\,\mathrm{d}u \right)^{1/2}, \tag{40}$$

which is the exact value in the limit $\beta \rightarrow \infty$. On the other hand, for $\beta < 2$ the reaction term is concave and the speed of the flame is given by the KPP value

$$c_{\mathrm{KPP}} = 2\sqrt{f'(0)}. \tag{41}$$

Realistic values of β lie between these two extremes. Corrections to the ZFK formula have been obtained by means of asymptotic expansions in the parameter $1/\beta$ [29]. Often the prescription has been [4] to take the larger value between c_{ZFK} (or its corrections) and c_{KPP} as the best approximation to the correct value of the speed. We have used the variational principle given by Theorem 1 above to compute several simple analytic formulas that reproduce the numerical value of the speed of the flame for a wide range of the parameter β [30]. We have also used the variational principle (1) to prove that c_{ZFK} is always a lower bound for any reaction term of type A [19,30] (a different proof of this fact has been given directly from the ordinary differential equation by Berestycki and Nirenberg [31]). For completeness we reproduce here the proof of this lower bound.

Theorem 3.1 ([19,30,31]). *For any reaction term $f(u)$ of type A, the selected speed of propagation of sufficiently localized initial conditions satisfies,*

$$c^* \geq c_{\mathrm{ZFK}} \equiv \left(2\int_0^1 f(u)\mathrm{d}u\right)^{1/2}, \tag{42}$$

Proof: Choose as a trial function,

$$g(q) = \sqrt{2\int_q^1 f(s)\mathrm{d}s}, \tag{43}$$

in Eq. (5). Clearly this function is in $\mathcal{E}$.

With this choice we obtain

$$\int_0^1 \sqrt{fgh}\mathrm{d}u = \int_0^1 f(u)\mathrm{d}u, \tag{44}$$

and we have that

$$\int_0^1 g(u)\mathrm{d}u = -\int_0^1 g'(u)u\mathrm{d}u \leq -\int_0^1 g'(u)\mathrm{d}u = g(0), \tag{45}$$

since $g(1) = 0$. Replacing Eqs. (44) and (45) in Eq. (5) we obtain,

$$c \geq 2\frac{\int_0^1 f(u)\mathrm{d}u}{g(0)} = \sqrt{2\int_0^1 f(u)\mathrm{d}u} = c_{\mathrm{ZFK}}, \tag{46}$$

i.e. the minimal speed is always greater than or equal to the ZFK value. □

Using the variational principle one can get an approximation to the minimal speed of the flame, which is a much better approximation than the c_{ZFK} value for intermediate values of the Zeldovich parameter.

Defining, $r(x) = \int_x^1 f(u)\mathrm{d}u$, taking $g = r^n$ as a trial function in Eq. (5), and optimizing in n, we are led to the following lower bound on the minimal speed [30]

$$c \geq \frac{4\sqrt{n}}{2n+1}\frac{\left(\int_0^1 f(u)\mathrm{d}u\right)^{n+1/2}}{\left(\int_0^1 uf(u)\mathrm{d}u\right)^2}, \tag{47}$$

for any $n \in (1/2, 1)$ and for any reaction term of type A. The n that maximizes this lower bound is either

$$n = \frac{1 - \log(\gamma) - \sqrt{[\log(\gamma) - 1]^2 - 4\log(\gamma)}}{4\log(\gamma)}, \tag{48}$$

when the right side of Eq. (48) is real, where

$$\gamma = \frac{\int_0^1 f(u)\mathrm{d}u}{\int_0^1 uf(u)\mathrm{d}u},$$

or $n = 1$ otherwise [30].

4. Minimal speed of fronts for reaction–convection–diffusion equations

In many processes, in addition to diffusion, motion can also be due to advection or convection. Nonlinear advection terms arise naturally in the motion of chemotactic cells. In a simple 1D model, denoted by ρ the density of bacteria, chemotactic to a single chemical element of concentration $s(x,t)$ the density evolves according to

$$\rho_t = [D\rho_x - \rho\xi s_x]_x + f(\rho), \tag{49}$$

where diffusion, chemotaxis and growth have been considered. There is some evidence [32] that, in certain cases, the rate of chemical consumption is due mainly to the ability of the bacteria to consume it. In that case,

$$s_t = -k\rho,$$

where diffusion of the chemical has been neglected (arguments to justify this approximation, together with the choice of constants D and ξ are given in Ref. [32]). If one looks for traveling-wave solutions, $s = s(x - ct)$, and $\rho = \rho(x - ct)$, then $s_t = -cs_x$, and thus, $s_x = k\rho/c$, and the problem reduces to a single differential equation for the density ρ, namely

$$\rho_t = D\rho_{xx} - \xi\tfrac{k}{c}(\rho^2)_x + f(\rho). \tag{50}$$

For a discussion about the recent literature on the subject, see, e.g. Ref. [20] and references therein.

Motivated by the previous model, in this section we will consider the equation with a general convective term that, suitably scaled, we write as

$$u_t + \mu\phi(u)u_x = u_{xx} + f(u), \tag{51}$$

where the reaction term is of type A. The function $\phi(u) \in C^1([0,1])$. Without loss of generality we may assume $\phi(0) = 0$, since otherwise only a uniform shift in the speed is introduced. The parameter μ is positive. For Eq. (51), the existence of monotonic decaying traveling fronts, $u(x - ct)$ for any wave speed greater than a critical value c^* was proven recently by Malaguti and Marcelli [33]. In Ref. [33], the following estimate on c^* was derived,

$$2\sqrt{f'(0)} \leq c^* \leq \sqrt{\sup_{u\in[0,1]} \frac{f(u)}{u}} + \max_{u\in[0,1]} \mu\phi(u). \tag{52}$$

Analogous results for density-dependent diffusion have also been established in Ref. [33]. The convergence of some initial conditions to a monotonic traveling front has been proven by Crooks [34] for systems for which the minimal speed is greater than the linear value $c_{\mathrm{KPP}} = 2\sqrt{f'(0)}$.

We have recently derived a variational characterization for the minimal speed c^* of monotonic traveling front solutions of Eq. (51) [20]. Let

$$I(g) = \frac{\int_0^1 \left(2\sqrt{f(u)g(u)[-g'(u)]} + \mu\phi(u)g(u)\right)\mathrm{d}u}{\int_0^1 g(u)\mathrm{d}u} \tag{53}$$

defined over the set S of positive, monotonic decreasing functions $g(u)$, in $C^1([0,1])$, with $g(1) = 0$. Then we have

Theorem 4.1 ([20])

$$c^* = \sup_{g\in S} I(g). \tag{54}$$

Remarks 4.2 (i) Using the variational principle (54), Jensen's inequality and integration by parts one can derive the upper bound Eq. (52) [20]. (ii) From the variational principle Eq. (54) it is also possible to show that a sufficient condition for c^* to be equal to the linear value c_{KPP} is

$$\frac{f''(u)}{\sqrt{f'(0)}} + \mu\phi'(u) < 0,$$

for all $u \in (0,1]$ [20].

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