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Counterexample to a conjecture of Goriely for the speed of fronts of the reaction-diffusion equation

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In a recent paper, Goriely [A. Goriely, Phys. Rev. Lett. **75**, 2047 (1995)] considers the one-dimensional scalar reaction-diffusion equation $u_t = u_{xx} + f(u)$, with a polynomial reaction term $f(u)$, and conjectures the existence of a relation between a global resonance of the Hamiltonian system $u_{xx} + f(u) = 0$ and the asymptotic speed of propagation of fronts of the reaction-diffusion equation. Based on this conjecture an explicit expression for the speed of the front is given. We give a counterexample to this conjecture and present evidence indicative that it holds only for a particular class of exactly solvable problems. [S1063-651X(97)11402-7]

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The one-dimensional scalar reaction-diffusion equation

$$u_t = u_{xx} + f(u), \tag{1}$$

with $f(0) = f(u_+) = 0$ has been the subject of much study, not only because it models different phenomena [1–3], but also because it is the simplest reaction-diffusion equation for which rigorous results can be obtained [3–11]. Depending on the situation being considered the reaction term $f(u)$ satisfies additional properties. It has been shown for different classes of reaction terms that suitable initial conditions $u(x,0)$ evolve in time into a monotonic front joining the state $u = u_+$ to $u = 0$. The asymptotic speed at which the front travels is the minimal speed for which a traveling monotonic front $u(z) = u(x - ct)$ exists [5,7]. Traveling fronts are a solution of the ordinary differential equation $u_{zz} + cu_z + f(u) = 0$. In the present case we shall be concerned with two types of reaction terms, the classical case $f > 0$ in $(0, u_+)$ with $f'(0) > 0$ and the bistable case $f < 0$ in $(0, a)$, $f > 0$ in (a, u_+) with $\int_0^{u_+} f > 0$ and $f'(0) < 0$. In the classical case there is a continuum of speeds $c \geqslant c^*$ for which monotonic fronts exist. The system evolves into the front of speed c^*. In the bistable case there is a unique isolated value of the speed c^* for which a monotonic front exists, the system evolves into this front. The problem is to determine the speed of propagation of the front. In the classical case, if in addition $f'(0) > f(u)/u$ the speed of propagation c^* is the so called linear or Kolmogorov-Petrovsky-Piskunov (KPP) value $c_{KPP} = 2\sqrt{f'(0)}$ [4]. In the other cases (as well as in the bistable case) there exist variational principles, both local and integral, from which the speed can be calculated with any desired accuracy for arbitrary f [3,6,10,11].

In a recent paper [12] Goriely proposes a new method for the determination of the speed. Based on an observed property of some exactly solvable cases, namely, reaction terms of the form $f(u) = \mu u + \nu u^n - u^{2n-1}$, he conjectures that for polynomial reaction terms of the form

$$f(u) = \mu u + g(u), \tag{2}$$

where $g(0) = g'(0) = 0$ and with the polynomial g independent of μ, the speed of the front can be calculated from the knowledge of the heteroclinic orbit of the Hamiltonian system $u_{zz} + f(u) = 0$. This property of these solvable cases had not been observed before. In this Brief Report we show by means of a counterexample that this conjecture is not true, in general, for the above class of polynomial reaction terms. In order to assess its validity we consider simple reaction terms of the form $f(u) = \mu u + u^n - u^m$ and study the neighborhood of the Hamiltonian case. Comparison of results obtained directly from the equation differ from those obtained from Goriely's conjecture indicating that the conjecture does not hold except for the special case $m = 2n - 1$.

For the sake of clarity we state the conjecture here. The conjecture makes use of the fact that the front approaches the equilibrium state $u = 0$ as $e^{\lambda_- z}$, a well established fact, and approaches the equilibrium point $u = u_+$ as $u = u_+ - Le^{\gamma_+ z}$, an assumption which is not always satisfied. Then the global resonance, defined as

$$\delta = -\gamma_+/\lambda_- \tag{3}$$

is conjectured to be a constant, for a general class of polynomial reaction terms, at all values of μ for which the nonlinear front exists. Explicit expressions are known for the rates of approach γ_+ and λ_- in terms of c and f therefore, if δ can be calculated at any point, then an analytic formula for the speed can be obtained. There is such a point where it can be calculated, and that is the point at which $c = 0$ and the system is Hamiltonian. There is a unique value $\mu < 0$ for which such a front exists (we shall label it as μ_h and the corresponding equilibrium point as u_h), and therefore the speed is completely determined. The speed is conjectured to be

$$c_{gor} = \frac{\mu\delta^2 - f'(u_+)}{\sqrt{-\delta(1+\delta)[f'(u_+) + \delta\mu]}}, \tag{4}$$

with a constant value for δ. Below we give a counterexample to this conjecture. The main ingredient in constructing a counterexample is to observe that the expression for the speed (4) cannot hold if $|f'(u_+)|$ is sufficiently small since the denominator becomes complex. Moreover, for a general polynomial reaction term, as μ is varied, zeroes of the function $f(u)$ may appear or disappear leading to discontinuities

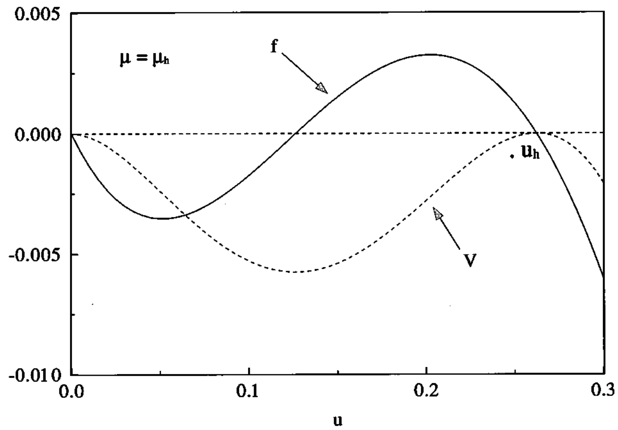

FIG. 1. Graph of the reaction term f and the corresponding scaled potential at the value of μ for which the speed of the front vanishes and the system is Hamiltonian.

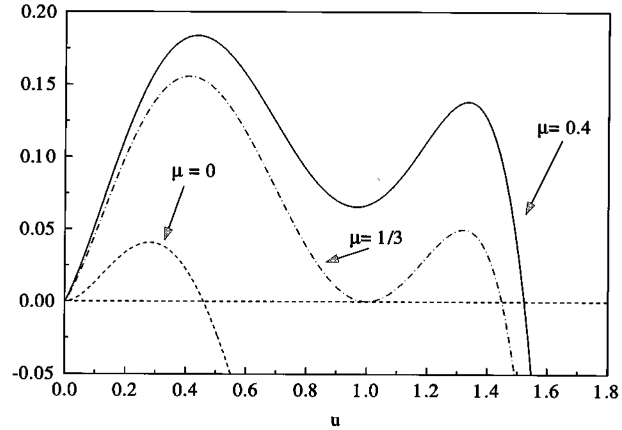

FIG. 2. Graph of the reaction term at different values of μ. The value of the stable point increases with μ until μ reaches 1/3. A discontinuous jump in the stable point occurs at that value.

in $f'(u_+)$ but not to discontinuities in the speed. We consider simpler reaction terms of the form $f(u)=\mu u+u^n-u^m$ with $n<m$. In this case the smallest positive zero u_+ varies continuously with μ and does not disappear as μ increases. In order to assess the validity of the conjecture we calculate the derivative $dc/d\mu$ at μ_H. The derivative obtained directly from the equation differs from the one obtained using Goriely's expression except in the solvable case $m=2n-1$. This is strongly indicative that the conjecture states a property of these particular systems.

Consider the reaction term $f(u)=\mu u+2u^2-7u^3+\frac{20}{3}u^4-2u^5$. This is of the form $f(u)=\mu u+g(u)$ where the polynomial $g(u)=2u^2-7u^3+20u^4/3-2u^5$ satisfies the properties $g(0)=g'(0)=0$ and is independent of μ as requested by the conjecture. For the Hamiltonian system $u_{zz}+\mu u+2u^2-7u^3+\frac{20}{3}u^4-2u^5=0$ a heteroclinic orbit joining two equilibrium points exists at the value $\mu=\mu_h=-0.153\,897$. In Fig. 1 the reaction term $f(u)$ is shown together with the (scaled) potential. It is clear that a heteroclinic solution joining the point $u=0$ to $u_+=u_h=0.262\,156$ exists. In this case the resonance δ can be calculated. Its value is given by $\delta=\delta_h=\sqrt{f'(u_h)/\mu_h}=0.865\,558$.

Let us now consider the propagating fronts which are a solution of $u_{zz}+cu_z+\mu u+2u^2-7u^3+\frac{20}{3}u^4-2u^5=0$. Before giving the results of the numerical and analytical calculations, we show the plot of the function f at several values of μ, which will make clear the numerical and analytical results that follow. As μ increases the equilibrium point u_+ increases until at $\mu=1/3$ it reaches the value $u_+=1$, where $f'=0$. Above this value of μ there is a discontinuous jump in u_+, the front joins the origin $u=0$ to a new fixed point which corresponds to a different root of the polynomial $f(u)$. In Fig. 2 we show the function f at different values of μ. At $\mu=1/3$ the fixed point $u_+=1$ and the derivative $f'(u_+)=0$. At $\mu=0.4$, we see that the value of u_+ is now the new root of f which did not exist at low values of μ.

First we describe the results of the numerical integrations of the initial value problem for Eq. (1) with sufficiently localized initial value perturbations $u(x,0)$. In Fig. 3 we show the asymptotic speed of the front as a function of μ. We see that even though the value of u_+ is discontinuous, the speed is a continuous function of μ. The solid line shows the numerical results and the dotted-dashed line corresponds to the linear or KPP value $2\sqrt{\mu}$. The dashed line is the speed predicted by the conjecture Eq. (4) with $\delta=0.865\,558$. The value $c_{\rm Gor}$ gives a good approximation near μ_H (where it is exact by construction), it departs from the correct value at larger μ and predicts erroneously the transition to the KPP regime. As μ approaches 1/3 the value $c_{\rm Gor}$ is no longer applicable as it predicts a complex value for the speed. Above $\mu=1/3$ the value predicted by c_{gor} is well above the observed value. In conclusion, from the numerical integration it follows that for the reaction term that we have considered the conjecture is not valid and δ is not a constant along the curve $c(\mu)$. Therefore we have calculated the value of δ along the curve. Once the speed is obtained numerically the value of δ is then computed from Eq. (3) which can be expressed as [12]

$$\delta=\frac{-c+\sqrt{c^2-4f'(u_+)}}{c+\sqrt{c^2-4f'(0)}}. \tag{5}$$

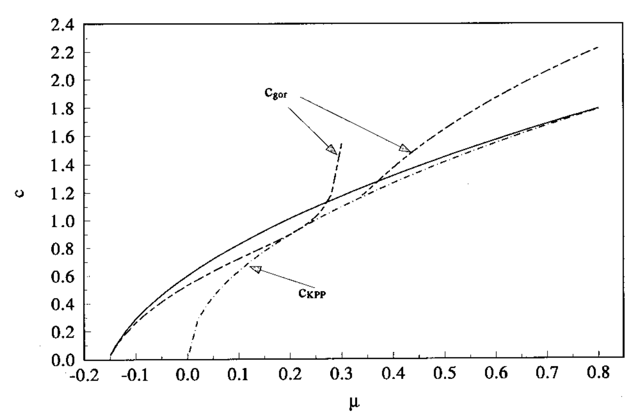

FIG. 3. Graph of the speed obtained from the numerical integration of the initial value problem. The speed of the front is a continuous function of μ. In the range of μ shown the speed is greater than the linear or KPP value.

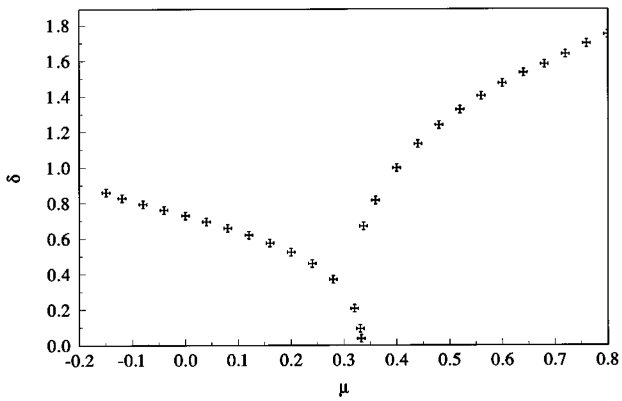

FIG. 4. Value of the resonance δ as a function of μ obtained from the numerical integrations.

The graph of δ as a function of μ is shown in Fig. 4. At $\mu=\mu_h$ it adopts the analytically calculated value from the Hamiltonian case, decreases to a value $\delta=0$ at $\mu=1/3$, jumps discontinuously to a larger value and increases from there on. This discontinuity is due to the discontinuity in u_+ and of $f'(u_+)$. At the value of $\mu=1/3$ where $f'(u_+)=0$ it is evident from Eq. (5) that $\delta=0$. As we will show below, at this value of μ the speed and the asymptotic behavior for the front can be calculated analytically and it is found that the front does not approach the fixed point $u_+=1$ exponentially. We next show that at $\mu=1/3$ the front approaches $u=1$ as $u\sim 1-A/z$.

By making use of variational principles [6,10] with suitable trial functions, one can show that $\sqrt{3/2}\leqslant c\leqslant\sqrt{3/2}$ so that the speed is exactly 3/2, which confirms the numerical results. The exact value of the speed can be obtained analytically from the variational principles due to the fact that for $\mu=1/3$ the derivative of the front can be calculated exactly. The derivative of the front as a function of u, $p(u)=-du/dz$ satisfies the equation $p(u)p'(u)-cp(u)+f(u)=0$ and the exact solution at $\mu=1/3$ is given by $p(u)=\sqrt{2/3}u(1-u)^2$. With this expression for p we may calculate the approach to the fixed point $u=1$. Near $u=1$, $p\sim\sqrt{2/3}(1-u)^2$ so that $du/dz\sim-\sqrt{(2/3)}(1-u)^2$ from where it follows that $u(z)\sim 1-\sqrt{(3/2)}(1/z)$. We see then that at this point $\delta=0$ since the rate of approach is not exponential but algebraic. Having seen numerically and analytically that δ is not constant along the solution in this example we conclude that the the conjecture does not hold for general polynomials of the form given by Eq. (2).

Here, in order to establish the possible range of validity of the conjecture, we consider a simpler class of polynomials for which the stable point u_+ varies continuously with μ. We shall analyze the neighborhood of the Hamiltonian case by calculating the derivative $dc/d\mu$ at μ_h directly from the equation and compare it with the result that follows from Goriely's expression for the speed. These two are found to differ, except in the special class of exactly solvable systems $f(u)=\mu u+u^n-u^{2n-1}$.

Traveling front solutions $u(x-ct)$ of Eq. (1) satisfy the ordinary differential equation $u_{zz}+cu_z+f(u)=0$ from where it follows, multiplying by u_z and integrating,

$$c\int_{-\infty}^{\infty}u_z^2dz=\int_0^{u_+}f(u)du, \tag{6}$$

where we have made use of the fact that for the front $u'<0$, so that u can be used as the independent variable in the term involving the reaction f. Since f and, hence, u_+ and c depend on μ, taking the derivative with respect to μ of Eq. (6) and evaluating at μ_h we obtain

$$\left.\frac{dc}{d\mu}\right|_{\mu_h}=\left.\frac{\int_0^{u_+}(\partial f/\partial\mu)du}{\int_{-\infty}^{\infty}u_z^2dz}\right|_{\mu_h}, \tag{7}$$

where we have used that $c=0$ at $\mu=\mu_h$ and that $f(u_+)=0$. Since we will consider terms of the form $f(u)=\mu u+g(u)$, the integral in the numerator can be done, it yields $u_+^2/2$. The integral in the denominator can be expressed in terms of the potential $V(u)$ as follows. The front in the Hamiltonian case is the heteroclinic solution of zero energy (see Fig. 1) of the equation $u_{zz}+f(u)=0$. Therefore, at μ_h, $u_z^2/2+V(u)=0$ and we finally obtain

$$\left.\frac{dc}{d\mu}\right|_{\mu_h}=\left.\frac{u_+^2/2}{\int_0^{u_+}\sqrt{-2V(u)}du}\right|_{\mu_h}. \tag{8}$$

This expression gives the exact derivative of c at μ_h.

Now we calculate the derivative obtained from Goriely's formula Eq. (4). Again, using $c=0$ at μ_h we obtain

$$\left.\frac{dc_{gor}}{d\mu}\right|_{\mu_h}=\frac{\delta^2-[1-(u_+/f'(u_+))\partial^2g(u_+)/\partial u^2]}{\sqrt{-\delta(1+\delta)[f'(u_+)+\delta\mu]}}, \tag{9}$$

where we used that $\partial u_+/\partial\mu=-u_+/f'(u_+)$.

We shall now compare the results for simple polynomials. First consider the exactly solvable case $f(u)=\mu u+u^2-u^3$. For this reaction term $u_+=2/3$, $\mu_h=-2/9$, $f'(u_+)=-2/9$, $\delta=1$, and $g''(u_+)=-2$. We obtain that the exact derivative coincides with that obtained from Goriely's expression, they yield $9/\sqrt{2}$. This was already guaranteed since the conjecture is based on a property of these exactly solvable systems.

Next consider the reaction term $f(u)=\mu u+u^4-u^5$. The potential is given by $V(u)=\mu u^2/2+u^5/5-u^6/6$. We find $u_+=9/10$, $\mu_h=-9^3/10^4$, $f'(u_+)=-6\times 9^3/10^4$, $\delta=\sqrt{6}$ and $g''(u_+)=-6\times 9^2/10^2$. From the exact expression Eq.(8) we obtain

$$\left.\frac{dc}{d\mu}\right|_{\mu_h}$$

$$=\frac{300}{-15+30\sqrt{6}+7\sqrt{3}\ln(-4+3\sqrt{2})-7\sqrt{3}\ln(-1+\sqrt{3})}$$

$$\approx 6.652\,45$$

TABLE I. Comparison of the derivatives $dc/d\mu$ at $\mu=\mu_h$ for $f(u)=\mu u+u^n-u^5$ for different values of n.

	$n=2$	$n=3$	$n=4$
$dc/d\mu$ (Gor)	4.184	4.619	6.575
$dc/d\mu$ (exact)	3.990	4.619	6.652

TABLE II. Comparison of the derivatives $dc/d\mu$ at $\mu=\mu_h$ for $f(u)=\mu u+u^n-u^7$ for different values of n.

	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
$dc/d\mu$ (Gor)	3.690	3.630	4.167	5.238	7.681
$dc/d\mu$ (exact)	3.385	3.554	4.167	5.280	7.763

and from Goriely's expression we obtain

$$\left.\frac{dc_{gor}}{d\mu}\right|_{\mu_h}=\frac{500}{9(6+\sqrt{6})}\approx 6.575\,02,$$

which is close numerically but not exact. The example we have just considered was presented as one in which the conjecture seemed to hold. There is close numerical agreement in this case, but it is not exact as it should be. We have calculated the slope of the speed at μ_h for reaction terms of the form $f(u)=\mu u+u^n-u^m$ for different values of n and m. The results are shown in Tables I and II. Even though the values are close for some exponents they differ significantly for others. Exact agreement is found only when $m=2n-1$, leading us to conclude that the conjecture is a characteristic of these special systems.

In conclusion, we have seen by means of a counterexample that the conjecture put forward, that relates certain properties of the Hamiltonian system $u_{zz}+f(u)=0$ with the speed of the front solution of $u_{zz}+cu_z+f(u)=0$, is not satisfied by general polynomial reaction terms $f(u)$. Consideration of a restricted class of polynomial reaction terms enables us to calculate analytically the slope of the speed at the Hamiltonian case. It is found that the slope predicted from Goriely's formula for the speed coincides with the exact value, only, for the exactly solvable cases, this is strongly indicative that the conjecture is a property of the special systems where it was observed, and does not hold for more general reaction terms.

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