Nonuniform reaction rate distribution for the generalized Fisher equation: Ignition ahead of the reaction front

Sergei Fedotov*
Department of Mathematics, UMIST, Manchester M60 1QD, United Kingdom
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We have addressed the problem of wavefront propagation for the generalized Fisher equation involving diffusion transport with a finite velocity and a spatially nonuniform reaction rate. We have considered in detail the phenomenon of wavefront jump or ignition ahead of the reaction front for a piecewise constant reaction rate. By using a relativistic mechanics technique based on the principle of least action we have found the criterion under which the ignition phenomenon happens and the time of appearance of the new front ahead of the initial reaction front. [S1063-651X(99)16810-7]

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I. INTRODUCTION

The solution of the classical Fisher equation with frontlike initial condition converges to a traveling wave solution in the long-time limit [1–4]. It is well known that the rate u at which the wave propagates can be determined exactly, namely, $u=\sqrt{4DU}$, where D is the diffusion coefficient and U is the reaction rate coefficient. The basic disadvantage of this formula is that it gives us an infinite speed of wave propagation when the chemical rate becomes very fast. Clearly this contradicts the simple physical fact that the speed u should not exceed the propagation rate of the real transport process. This contradiction requires the modification of the transport process based on the diffusion approximation by using some sort of hyperbolic terms [5–7] and this has been the focus of several recent studies [8–17].

It should be noted that there is another way to overcome this problem of the structural stability [18,19] by the introduction of a cutoff on the reaction term in the leading edge of the front profile [20,21]. A very interesting result has been found that if we replace the reaction rate by zero whenever the scalar field is less than a cutoff ϵ the effect on the propagation rate is very strong. The shift in propagating velocity is found to be of the form $K\,(\ln\epsilon)^{-2}$ for the small values of ϵ.

The basic problem with the classical Fisher equation in terms of the transport process is that it is described by diffusion approximation and the rate at which the wave propagates throughout the reaction-diffusion system can be overestimated. This may be explained by the physical fact that the density field predicted by the diffusion approximation (infinite speed of propagation) has higher tails than the density of real transport process [5,6,22,23]. Recently [12,13] we introduced a relativistic mechanics technique which allows us to analyze the reaction front dynamics for the generalized Fisher equation involving the diffusion with a finite velocity in terms of the Hamilton-Jacobi equation for a relativistic particle in a potential field. It is the purpose of this paper to use this technique for analyzing the case when the reaction rate coefficient is a function of the space coordinate. It was Freidlin [3,4] who discovered that for nonuniform spatial distribution of the chemical rate the wave front for the classical Fisher equation may have a jump. The basic idea is that if the chemical rate coefficient U is a rapidly growing function in the direction of wave propagation, ignition may take place ahead of the wavefront. The aim of this paper is to find out whether or not this phenomenon still exists in the case of the generalized Fisher equation involving a diffusion with finite velocity and, if so, to determine the basic characteristics of it, namely, the circumstances under which this phenomenon might happen and the ignition time or the time of appearance of the ''new source'' ahead of the wavefront. It is clear from a physical point of view that this phenomenon ceases to exist in the case of very fast chemical reaction when the reaction front moves with the maximal possible speed [12,13].

It should be also noted that we consider here only the case of front propagation into an unstable state. The basic reason is that the phenomenon of the reaction front jump ceases to exist for a trigger wave, that is, in the case of propagation into a metastable state [3,4].

II. STATEMENT OF THE PROBLEM

In this paper we give a detailed description of the phenomenon of ignition ahead of the reaction front in the simplest nontrivial case of piecewise constant reaction rate. The generalized Fisher equation after hyperbolic rescaling in one space dimension may be written as follows [12,13]:

$$\frac{\partial\rho^{\varepsilon}}{\partial t}=\frac{D}{\tau}\int_0^t \exp\left(-\frac{t-s}{\varepsilon\tau}\right)\frac{\partial^2\rho^{\varepsilon}}{\partial x^2}(s,x)\,ds + \frac{U(x)}{\varepsilon}\rho^{\varepsilon}(1-\rho^{\varepsilon}),\quad x\in R^1 \tag{1}$$

where D is the diffusion coefficient, $U(x)$ is the spatially nonuniform reaction rate coefficient, τ is the relaxation time, and ε is the small parameter describing the slow variation of reaction rate in space. It is assumed that the scalar field ρ^{ε} varies from 0 to 1.

*Electronic address: sergei.fedotov@umist.ac.uk

In fact we can also consider the general reaction rate term of the Kolmogorov-Petrovskii-Piskunov type [1–4]

$$\frac{U(x)}{\varepsilon}\rho^{\varepsilon}f(\rho^{\varepsilon}),$$

where the nonlinear function $f(\rho)$ has the properties

$$\max_{\rho\in[0,1]} f(\rho)=f(0)=1, \quad f(0)=0.$$

However, since the major feature of the front propagation into an unstable state is that the dynamics of reaction front is determined by the processes taking place in the leading edge of the front profile [1–4,24], the main results can be obtained by using the simplified kinetics

$$\frac{U(x)}{\varepsilon}\rho^{\varepsilon}(1-\rho^{\varepsilon})$$

without any restriction of a degree of generality.

For the sake of simplicity we consider the initial distribution of the scalar field in the form of a step function

$$\rho(0,x)=H(x), \tag{2}$$

where $H(x)$ is a Heaviside function $H(x)=1$ for $x\leqslant 0$ and $H(x)=0$ for $x>0$. For an arbitrary initial condition we have so-called problem of velocity selection [1–4]. Let us discuss this in more details. The choice of the initial condition in terms of the front-like function (2) ensures the selection of the minimum propagation speed. If, for example, the initial distribution has the exponential form

$$\rho(0,x)=\begin{cases}1, & \text{if } x\leqslant 0\\ \exp(-\alpha x), & \text{if } x>0,\end{cases}$$

then for the classical Fisher equation the propagation rate u can be written as [3,4]

$$u=\begin{cases}\sqrt{2D}\left(\dfrac{U}{\alpha}+\dfrac{\alpha}{2}\right), & \text{if } \alpha<\sqrt{2U}\\ \sqrt{4DU}, & \text{if } \alpha\geqslant\sqrt{2U}.\end{cases}$$

It follows from here that the propagation rate can vary from the minimum propagation speed $\sqrt{4DU}$ to infinity when $\alpha\to 0$. That is why in this paper we choose the initial condition in the form of step function (2) to concentrate on the phenomenon of reaction front jump.

We assume that the reaction rate $U(x)$ is piecewise constant such that

$$U(x)=\begin{cases}U_1, & \text{if } x<h\\ U_2, & \text{if } x\geqslant h\end{cases} \quad U_2>U_1. \tag{3}$$

Our purpose is to analyze the behavior of the solution of the initial value problem (1) and (2) in the limit $\varepsilon\to 0$. It is clear from (1) that this limit corresponds to the case when the reaction rate is very fast (ε appears in the denominator) and the transport process is very slow. When $\varepsilon\to 0$ the nonlinear term becomes dominant and therefore the solution ρ^{ε} can take only two values 0 and 1 everywhere except the narrow region in space where the diffusion and nonlinear terms are balanced. Those regions can be regarded as the reaction fronts and our aim is to find the location of the reaction fronts and the rate at which they move.

Since $\rho^{\varepsilon}(t,x)$ is a scalar field varying from 0 to 1, we can make an exponential transformation

$$\rho^{\varepsilon}(t,x)=\exp\left(-\frac{G^{\varepsilon}(t,x)}{\varepsilon}\right), \quad G^{\varepsilon}(t,x)\geqslant 0. \tag{4}$$

such that the limiting function

$$G(t,x)=\lim_{\varepsilon\to 0} G^{\varepsilon}(t,x) \tag{5}$$

varying from 0 to ∞ determines the location of the reaction fronts $S=\{x\in R^1: G(t,x)=0\}$ [12,13,25–27].

It turns out that the function $G(t,x)$ is the solution of the relativistic Hamilton-Jacobi equation for a charge particle ($e=1$) with the mass $m(x)$ moving in the potential field $\varphi(x)$ [12,13]

$$\frac{\partial G}{\partial t}+\sqrt{m^2(x)c^4+c^2\left(\frac{\partial G}{\partial x}\right)^2}+\varphi(x)=0, \quad [G(t,x)>0], \tag{6}$$

where the speed of light c, the mass $m(x)$ depending on the space coordinate x and potential field $\varphi(x)$ can be determined through the phenomenological parameters D, τ, and $U(x)$ as follows:

$$c^2=\frac{D}{\tau}, \quad \varphi(x)=\frac{1}{2}\left(U(x)-\frac{1}{\tau}\right), \quad m(x)=\frac{\tau}{2D}\left(U(x)+\frac{1}{\tau}\right). \tag{7}$$

The advantage of an analogy with the relativistic mechanics is that we can find the solution of (6) as follows [28]

$$G(t,x)=\min\left\{\int_0^t L\,ds: \quad x(0)=x, \quad x(t)=0\right\},$$

$$G(t,x)>0, \tag{8}$$

where the Lagrangian L has the form [28]

$$L=-m(x)c^2\sqrt{1-\frac{1}{c^2}\left(\frac{dx}{ds}\right)^2}-\varphi(x) \tag{9}$$

and

$$\varphi(x)=\begin{cases}\dfrac{1}{2}\left(U_1-\dfrac{1}{\tau}\right), & \text{if } x<h\\ \dfrac{1}{2}\left(U_2-\dfrac{1}{\tau}\right), & \text{if } x\geqslant h\end{cases} \tag{10}$$

$$m(x)=\begin{cases}\dfrac{\tau}{D}\left(U_1+\dfrac{1}{\tau}\right), & \text{if } x<h\\ \dfrac{\tau}{D}\left(U_2+\dfrac{1}{\tau}\right), & \text{if } x\geqslant h\end{cases}\qquad c^2=\frac{D}{\tau}. \tag{11}$$

It should be noted that we can also use in (8) the boundary conditions like $x(t)=x, x(0)=0$.

III. IGNITION AHEAD OF REACTION FRONT

Generally we expect that the solution $t=t(x)$ of the equation $G(t,x)=0$ is not a strictly monotonic function; this lack of monotonicity can be interpreted as the appearance of ignition points in the finite distance ahead of the moving initial reaction front [3,4]. A negative sign of the derivative dt/dx corresponds to the front moving from right to left. It is clear from a physical point of view that in the case of the piecewise reaction rate constant (3) the ignition might occur at the point h. Therefore, let us calculate the action functional for $x=h$. Since for $x(0)=h$, the chemical rate U_2 is greater than U_1 we may expect that it is preferable for the optimal trajectory $x(s)$ to spend some time t^* at the point $x=h$ and then to move to $x=0$. The Euler-Lagrange equation has a very simple form $d^2x/ds^2=0$ so that the optimal trajectory can be written as

$$x(s)=\begin{cases}h, & \text{if } 0\leqslant s\leqslant t^*\\ -\dfrac{hs}{t-t^*}+\dfrac{ht}{t-t^*}, & \text{if } t^*\leqslant s\leqslant t,\end{cases} \tag{12}$$

where the time t^* has to be found. Substituting this expression for $x(s)$ into the integral in (8), we obtain

$$G(t,h)=\tfrac{1}{2}\min_{t^*} V(t,h,t^*), \tag{13}$$

where the auxiliary function V is

$$V(t,h,t^*)=-2U_2t^*+\left(\frac{1}{\tau}-U_1\right)(t-t^*)-\left(\frac{1}{\tau}+U_1\right)\left((t-t^*)^2-\frac{\tau h^2}{D}\right)^{1/2}. \tag{14}$$

By equating $\partial V/\partial t^*$ to zero, we find the time t^* that minimizes V

$$t^*=t-\frac{h(1+2\tau U_2-\tau U_1)}{\sqrt{4D(U_2-U_1)(1+\tau U_2)}}. \tag{15}$$

After substituting (15) into (13) and (14) we obtain the expression for $G(t,h)$

$$G(t,h)=-U_2t+h\left(\frac{(U_2-U_1)(1+\tau U_2)}{D}\right)^{1/2}. \tag{16}$$

From the equation $G(t,h)=0$ we can find the ignition time

$$T=\frac{h}{U_2}\left(\frac{(U_2-U_1)(1+\tau U_2)}{D}\right)^{1/2}. \tag{17}$$

This is the time when the ignition takes place at the point $x=h$. After the ignition the new wavefront starts to move from $x=h$ in the both positive and negative directions.

It is interesting to consider the asymptotic limit of the ignition time T when the nondimensional parameter $U_2\to\infty$ (infinite chemical reaction rate). If the relaxation time $\tau=0$ as for the classical Fisher equation, the ignition time $T\to 0$ as $U_2^{-1/2}$. When $\tau\neq 0$ it follows from (16) that

$$\lim_{U_2\to\infty} T=h\left(\frac{\tau}{D}\right)^{1/2}=\frac{h}{c}>0.$$

Up to time T the old wavefront moves from the point $x=0$ with the rate

$$u_1=\frac{\sqrt{4DU_1}}{1+\tau U_1},\quad \tau U_1\leqslant 1$$

such that at $t=T$ its position L_T is

$$L_T=u_1T=\frac{2h\sqrt{U_1(U_2-U_1)(1+\tau U_2)}}{U_2(1+\tau U_1)}<h,\quad \tau U_1\leqslant 1.$$

The critical value of $U_2>U_1$ at which the phenomenon of wavefront jump ceases to exist can be found from the equality $L_T=h$, that is, $U_2^{cr}=2U_1/(1-\tau U_1)$. So the criterion for ignition ahead of the reaction front can be written as

$$U_2>U_2^{cr}=\frac{2U_1}{1-\tau U_1}. \tag{18}$$

Note that this value is larger than the corresponding one for the classical Fisher equation [3,4] and what is more it tends to infinity when $\tau U_1\to 1$. This result has a very clear physical meaning: the ignition phenomenon ceases to exist in the case $\tau U_1=1$ when the initial reaction front moves with the maximal possible speed $u=c=\sqrt{D/\tau}$.

IV. SUMMARY

We have analyzed the one-dimensional phenomenon of wavefront jump for the generalized Fisher equation involving diffusion transport with a finite velocity and a spatially nonuniform reaction rate. In the case of piecewise constant reaction rate we have found the ignition time when the appearance of a new front ahead of the initial reaction front takes place and the criterion under which this phenomenon might happen. We believe that the ignition phenomenon ahead of the reaction front might be of great value in combustion science where the Fisher equation can be used both for laminar flame propagation [29] and turbulent combustion [27,30,31]. It would also be interesting to explore the front jump phenomenon in the context of propagating magnetic fronts in disc dynamos when the local growth rate of magnetic field is the function of the space coordinate [32] and a forest fire model under the nonuniform reaction rate conditions [16].

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