Front Propagation into an Unstable State of Reaction-Transport Systems

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We studied the propagation of traveling fronts into an unstable state of the reaction-transport systems involving integral transport. By using a hyperbolic scaling procedure and singular perturbation techniques, we determined a Hamiltonian structure of reaction-transport equations. This structure allowed us to derive asymptotic formulas for the propagation rate of a reaction front. We showed that the macroscopic dynamics of the front are "nonuniversal" and depend on the choice of the underlying random walk model for the microscopic transport process.

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The problem of propagating fronts traveling into an unstable state of a reaction-transport system has attracted considerable interest in the past years, because of a large number of physical, chemical, and biological problems which can be treated in this framework [1–6]. A generic model which describes phenomena of this type is the Fisher-Kolmogorov-Petrovskii-Piskunov (FKPP) equation for a scalar field $\rho(t, x)$

$$\frac{\partial \rho}{\partial t} = D\,\frac{\partial^2 \rho}{\partial x^2} + U\rho(1 - \rho), \tag{1}$$

where D is a diffusion coefficient and U is a reaction rate parameter. The FKPP equation was originally introduced to investigate the spread of advantageous genes in a population [7]. Since then it has been widely used in other chemical and biological contexts to describe population growth and dispersion, the spread of epidemics [2,3], combustion waves [8], etc. The problem of front propagation into an unstable state can be considered as a fundamental problem in physics as well. Problems of this type arise in studies of the propagation of a vortex front in an unstable fluid flow [9], propagation of domain walls in liquid crystals [10], propagation of magnetic fronts in disk dynamos [11], as well as in models of aggregation and deposition [12].

It follows from Eq. (1) that the state $\rho = 0$ is unstable while the state $\rho = 1$ is stable. The basic question of interest is how fast front replacing the unstable state by the stable one will move. Dimensional analysis gives a simple answer to this question: the propagation rate u is proportional to $\sqrt{DU}$. The basic shortcoming of this estimation is that it gives an infinite speed of propagation when the chemical reaction becomes very fast ($U \to \infty$). Recently, there has been a tremendous amount of activity in extending the analysis based on (1) by introducing more realistic macroscopic descriptions of the transport processes [13–17]. The main motivation for this is that the diffusion approximation for transport admits an infinite speed of propagation. Because of this unphysical property of ordinary diffusion, the FKPP equation leads to the overestimation of the propagation speed of traveling fronts. It should be mentioned here that there is a lot of literature on the microscopic stochastic models for which the FKPP equation can be regarded as the mean-field approximation (see, for example, [18] and references therein).

In our opinion the fundamental deficiency of the FKPP equation is that it involves implicitly a long-time large-distance *parabolic scaling* while as far as the propagating fronts are concerned, the appropriate scaling must be a *hyperbolic* one. It is well known that the macroscopic transport process comes from the overall effect of many particles performing complex random movements. Classical diffusion is just an approximation for this transport in the long-time large-distance parabolic limit. What we are going to show here is that, in general, this approximation is not appropriate for the problems involving propagating fronts. The basis idea is that the kinetic term in (1) is very sensitive to the tails of a concentration/temperature profile, while these tails are typically "nonuniversal," "nondiffusional," and dependent on the microscopic details of transport process. Our purpose is to demonstrate that the macroscopic dynamics of the reaction front for a reaction-transport system are dependant on the choice of the underlying random walk model for transport processes.

In this Letter we choose an alternative description of reaction-transport processes; instead of equation (1) we consider two models: model A, discrete in time, and model B, continuous in time

$$\text{model } A: \qquad \rho(t + \tau, x) = \int_{-\infty}^{\infty} \rho(t, x + z)\varphi(z)\,dz + U(\varepsilon x)\tau\rho(t, x)[1 - \rho(t, x)], \tag{2}$$

$$\text{model } B: \qquad \frac{\partial \rho}{\partial t} = \lambda\left[\int_{-\infty}^{\infty} \rho(t, x + z)\varphi(z)\,dz - \rho(t, x)\right] + U(\varepsilon x)\rho(t, x)[1 - \rho(t, x)], \tag{3}$$

where the reaction rate parameter $U(\varepsilon x)$ is a slowly varying function of the space coordinate x; ε is a small parameter.

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These two equations provide a suitable coarse-grained description of the microscopic reaction and random spatial spread with long-range interaction modeled by the kernel $\varphi(z)$ [3]. We note that the integro-difference equations for the description of growth-dispersal phenomena have also been used in [13,19].

To understand the physical meaning of the parameters τ and λ and the function $\varphi(z)$ describing the transport process in (2) and (3), one can consider the following random walk models [20]. In model A the microscopic transport process can be viewed as follows: The particle moves at regular time intervals τ in the positive or negative direction in accordance with the equation $X(t + \tau) = X(t) + Z(t)$, $t = n\tau$, $n = 0, 1, 2, \ldots$, where the jumps $Z(t)$ are independent, identically distributed random variables with the probability density function given by $\varphi(z) = \frac{d}{dz}\Pr\{Z(t) \le z\}$. In model B the particle moves as follows: Starting at the point x it spends a random time ν and then undergoes a jump Z, where Z is a random variable having a given probability density function $\varphi(z)$, taking the point $x + Z$. Again it spends the random time ν and jumps and so on. The random time ν between the jumps is exponentially distributed with rate λ.

Now the problem is to obtain a traveling front for (2) and (3) and what is more to find the rate at which this front moves. To ensure the minimal speed of propagation, we consider here only the frontlike initial condition

$$\rho(0, x) = \theta(x), \tag{4}$$

where $\theta(x)$ is a Heaviside function: $\theta(x) = 1$ for $x \le 0$ and $\theta(x) = 0$ for $x > 0$.

Since the exact solutions of these integro-differential equations are not known, some sort of approximation is needed. The conventional way to simplify the problem is to approximate the integral term in (2) and (3) by the second derivative of ρ with respect to the spatial coordinate x and thereby to get the FKPP equation (1) (see, for example, [3]). In what follows we show that, in general, this approximation for a propagating front problem is not appropriate and may lead to unphysical results.

In this Letter we shall discuss in detail the particular case of both equations (2) and (3) when the kernel $\varphi(z)$ is

$$\varphi(z) = \frac{1}{2}\,\delta(z - a) + \frac{1}{2}\,\delta(z + a). \tag{5}$$

This case corresponds to the random walk model when the jumps Z can take only two values $-a$ or a with the equal probability $1/2$. Equation (2) takes the form

$$\rho(t + \tau, x) = \frac{1}{2}\,\rho(t, x + a) + \frac{1}{2}\,\rho(t, x - a) + U(\varepsilon x)\tau\rho(t, x)[1 - \rho(t, x)]. \tag{6}$$

This is a typical example of a coupled map lattice describing a logistic map and spatial diffusion. It has been extensively used in modeling traveling fronts and spatiotemporal chaos (see, for example, [21]). In the limits $a \to 0$ and $\tau \to 0$ such that $D = a^2/2\tau = \text{const}$, we can get from (6) the FKPP equation (1).

As far as traveling waves are concerned, the diffusion approximation is not adequate, in general, since in the limits $a \to 0$ and $\tau \to 0$ we should keep the velocity $v = a/\tau$ constant rather then $D = a^2/2\tau$. It is clear from a physical point of view that the velocity $v = a/\tau$ must be the maximum possible rate of front propagation.

The technique to be used in this Letter to obtain the traveling front for (2) and (3) involves a hyperbolic scaling, exponential transformation, and a Hamilton-Jacobi formalism. It is instructive first to consider the classical FKPP equation (1) with frontlike initial condition (4). The traditional way to deal with the FKPP equation is to find the traveling wave solution $\psi(x - ut)$ to the problem (1) and (4). However, we can treat Eq. (1) like one of a *mesoscopic* description of the reaction-transport process. The basic idea introduced by Freidlin [4] is that in the long-time large-distance *macroscopic* limit the detailed shape of the traveling wave is not important and therefore the problem of wave propagation is that of dynamics of a reaction front.

The hyperbolic scaling

$$t \to \frac{t}{\varepsilon}, \qquad x \to \frac{x}{\varepsilon} \qquad \varepsilon \ll 1 \tag{7}$$

leads to the Cauchy problem for a rescaled scalar field $\rho^\varepsilon(t, x) = \rho(t/\varepsilon, x/\varepsilon)$,

$$\frac{\partial\rho^\varepsilon}{\partial t} = \varepsilon D\,\frac{\partial^2\rho^\varepsilon}{\partial x^2} + \frac{1}{\varepsilon}\,U\rho^\varepsilon(1 - \rho^\varepsilon), \qquad \rho^\varepsilon(0, x) = \theta(x). \tag{8}$$

It is easy to see from this equation that in the limit $\varepsilon \to 0$ the reaction rate is very fast and the diffusion is very slow and therefore the solution ρ^ε takes only two values 0 and 1 as $\varepsilon \to 0$. The problem now is to derive the equation governing the position of the reaction front. If we now replace $\rho^\varepsilon(t, x)$ by an auxiliary field $G(t, x) \ge 0$ through the exponential transformation

$$\rho^\varepsilon(t, x) = \exp\left(-\frac{G(t, x)}{\varepsilon}\right), \tag{9}$$

substituting (9) into (8) yields, to leading order, the classical Hamilton-Jacobi equation $\partial G/\partial t + H(\partial G/\partial x) = 0$, with the Hamiltonian $H(p) = Dp^2 + U$. It follows from (9) that the location of the reaction front $x(t)$ can be determined from a very simple equation $G[t, x(t)] = 0$. The solution of the Hamilton-Jacobi equation is $G(t, x) = x^2/(4Dt) - Ut$, from which we easily find the position of the reaction front $x(t) = ut$, where the propagation rate $u = \sqrt{4DU}$.

Now we are in a position to investigate the problem of the reaction front propagation for the integro-differential Eqs. (2) and (3). We expect that after rescaling (7) the wave profile develops into the reaction front, that is, $\rho^\varepsilon(t, x) = \rho(t/\varepsilon, x/\varepsilon)$ tends to a unit step function $\theta(x - ut)$ as $\varepsilon \to 0$. Our goal now is to find a function $G(t, x)$ determining the position of the reaction front, that is $\lim_{\epsilon\to 0}\rho^\varepsilon(t, x) = 0$ when $G(t, x) > 0$ and

$\lim_{\epsilon\to 0}\rho^{\epsilon}(t,x) = 1$ when $G(t,x) = 0$. Again we seek a solution to rescaled Eqs. (2) and (3) in the exponential form (9), so that $G(t,x)$ obeys, to leading order in ϵ, the Hamilton-Jacobi equation

$$\frac{\partial G}{\partial t} + H\left(\frac{\partial G}{\partial x}, x\right) = 0, \tag{10}$$

where the respective Hamiltonians $H(p,x)$ are given by

$$\text{model } A: \qquad H(p,x) = \frac{1}{\tau}\ln\left[\int_{-\infty}^{\infty}\exp(zp)\varphi(z)\,dz + U(x)\tau\right], \tag{11}$$

$$\text{model } B: \qquad H(p,x) = \lambda\left[\int_{-\infty}^{\infty}\exp(zp)\varphi(z)\,dz - 1\right] + U(x). \tag{12}$$

This result is of particular importance as it shows that the reaction front dynamics for Eqs. (2) and (3) must be different than that for the classical FKPP equation (1). This follows from the fact that the Hamiltonians (11) and (12) governing the evolution of the action functional G and thereby the dynamics of the front are different from $H = Dp^2 + U$ corresponding to the FKPP equation.

When the kernel $\varphi(z)$ is a superposition of two delta functions as in (6) we have

$$\text{model } A: \qquad H(p,x) = \frac{1}{\tau}\ln[\cosh(ap) + U(x)\tau], \tag{13}$$

$$\text{model } B: \qquad H(p,x) = \lambda[\cosh(ap) - 1] + U(x). \tag{14}$$

Both Hamiltonians (13) and (14) involve the characteristic velocities a/τ and $a\lambda$ which must be infinite under the diffusion approximation. If $U = \text{const}$ it follows from a dimensional analysis that the front propagation speed u can be found from the nondimensional equations: $f_A(u\tau/a, U\tau) = 0$ for model A and $f_B(u/\lambda a, U/\lambda) = 0$ for model B, where f_A and f_B have to be determined. A fundamental difference between two models (13) and (14) with respect to propagating fronts is that discreteness in time of the model A leads to finite propagation rate, while model B admits an infinite speed of propagation in the limit of fast reaction ($U \to \infty$).

It is well known from classical mechanics that the solution of the Hamilton-Jacobi equation can be written as $G(t,x) = \int_0^t\{p(s)\,dx/ds - H[p(s),x(s)]\}\,ds$, where $x(s)$ and $p(s)$ satisfy the Hamilton equations $dx/ds = \partial H/\partial p$ and $dp/ds = -\partial H/\partial x$ with the conditions $x(0) = 0$, $x(t) = x$. The rate $u(t)$ at which the front moves can be found as follows: Let us differentiate $G[t,x(t)] = 0$ with respect to t. One can get $\partial G/\partial t + u(t)\partial G/\partial x = 0$ and therefore $u(t) = H/p$ since $\partial G/\partial t = -H$ and $\partial G/\partial x = p$.

To find an explicit expression for $G(t,x)$ and thereby the front position and its propagation speed, we restrict ourselves in this Letter to the case when the reaction rate parameter $U = \text{const}$. It should be noted here that if $U(x)$ is an increasing function of x it might induce an interesting phenomenon in which the front jumps [4,16]. Since the Hamiltonian H does not depend on the space coordinate and time, the Hamilton equations give us $H = \text{const}$ and $p = \text{const}$. By using the Hamilton equations we find $x(s) = s\partial H/\partial p$ and $\partial H/\partial p = x/t$. The action functional G corresponding to that of a free particle can be written as

$$G(t,x) = px - H(p)t. \tag{15}$$

Since the position of the reaction front is determined by the equation $G[t,x(t)] = 0$ and $x(t) = ut$, we can find two equations for the propagation rate u and the momentum p

$$u = \frac{\partial H}{\partial p}, \qquad \frac{\partial H}{\partial p} = \frac{H(p)}{p}. \tag{16}$$

By using the Hamiltonians from (11), (12), and (16), we can write down the explicit expressions for the front propagation rate u for both model A and model B

$$\text{model } A: \qquad u = \frac{1}{\tau}\,\frac{\int_{-\infty}^{\infty} z\exp(zp)\varphi(z)\,dz}{\int_{-\infty}^{\infty}\exp(zp)\varphi(z)\,dz + U\tau}, \tag{17}$$

$$\text{model } B: \qquad u = \lambda\int_{-\infty}^{\infty} z\exp(zp)\varphi(z)\,dz, \tag{18}$$

where the momentum p is a positive solution of the equation $pH'(p) = H(p)$.

With $\varphi(z)$ given by (5), we have [see the Hamiltonians (13) and (14)] the following expressions for the velocity u:

$$\text{model } A: \qquad u = \frac{a\sinh(ap)}{\tau[\cosh(ap) + U\tau]}, \tag{19}$$

$$\text{model } B: \qquad u = \lambda a\sinh(ap), \tag{20}$$

where p is a positive solution of $pH'(p) = H(p)$. An essential feature of the formula (19) is that in the limit $U \to \infty$ the propagation speed $u \to a/\tau = \text{const}$. This contrasts with the FKPP equation for which $u \to \infty$ as $U \to \infty$. However, model B (20) admits an infinite speed of propagation when $U \to \infty$ due to the property that the underlying random walk has of being continues in time.

Now let us discuss the main differences between the FKKP equation and models A and B. First, the explicit expression for the propagation rate u for models A and B cannot be found from simple dimensional analysis as it is in the FKPP equation case when u is proportional to $\sqrt{DU}$. The main physical reason for this is that models A and B involve the characteristic microscopic velocities, for example, a/τ and $a\lambda$. For the FKPP equation, the parabolic

scaling makes these velocities infinite. The divergence of the characteristic velocity of the microscopic transport process under parabolic scaling indicates that the details of these processes are irrelevant to the macroscopic behavior of the front. This observation suggests *the universality* of front propagation in terms of the FKPP equation. Notwithstanding the broad range of possible microscopic transport processes, the universal feature is observed under parabolic scaling. We can look at this reduction of a "complex" microscopic transport to a diffusion process as an application of the central limit theorem (CLT) [20]. The essence of the CLT and its importance for physics is that a Gaussian distribution can be regarded as an "attraction point" for the arbitrary random walks models after a parabolic scaling (see a discussion about CLT, universality, renormalization, etc., in a review [22]). The peculiar feature of nonlinear term in (1)–(3) is the sensitivity to the tails of the distribution of the scalar field ρ. However, it is well known that, in general, the CLT gives a poor approximation for the tails [20]. An appropriate tool for the estimation of the tails is the large deviation theory [4] that involves a hyperbolic scaling (7) suitable for the problem of front propagation. In this case we have a *nonuniversal* behavior, namely, the *macroscopic* dynamics of the front appears to be dependent on the choice of the statistics for the *microscopic* transport process.

Regarding the correspondence principle, model A and model B can be reduced to the FKPP equation in the case when we neglect the characteristic times τ and λ^{-1} compared to U^{-1}. As far as a reactive gas mixture is concerned, the parameter τU is very small indeed, since the mean free path time τ has a negligible duration in comparison with the average rate of chemical reaction U^{-1}. In this case, the FKPP equation can be considered as a good mean-field model for the front propagation. However, for turbulent reaction-transport processes [23] and biological applications such as population spread [13–15], the delay time τ or λ^{-1} might be the same order as U^{-1}. Model A and model B correspond to the cases when the microscopic transport processes are described by Markov random walks [20]. It should be stressed that our results can be applied to a much larger class of reaction-transport equations than the two models A and B we used in this Letter.

In summary, we have developed a Hamilton-Jacobi technique for the problem of wave propagation into an unstable state of the transport-reaction systems involving integral transport terms. We have derived *asymptotic* formulas for the speed of the reaction front. Our analysis does not involve the use of a diffusion approximation for the transport process. We have shown that the macroscopic dynamics of the reaction front for reaction-transport systems are dependent on the choice of the underlying random walk model for transport processes. The basic physical reason for this is that the unstable state of a transport-reaction system is very sensitive to the tails of a concentration/temperature profile, while these tails are typically nonuniversal, nondiffusional, and dependent on the microscopic details of transport processes.

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