Wave front for a reaction-diffusion system and relativistic Hamilton-Jacobi dynamics

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The problem of wave-front propagation for the n-dimensional reaction-diffusion system involving Kolmogorov-Petrovskii-Piskunov kinetics and the diffusion transport with a finite velocity has been considered. By using a scaling procedure we have given an asymptotic derivation of the equation governing the evolution of a reaction front in the long-time large-distance limit. It has been found that this equation is identical in form to the relativistic Hamilton-Jacobi equation. In the case of a constant value of chemical rate function we have derived exact formulas for the position of reaction front and the speed of propagation by using relativistic mechanics techniques. [S1063-651X(99)09005-4]

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I. INTRODUCTION

The Kolmogorov-Petrovskii-Piskunov (KPP) equation

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

and its various generalizations have attracted considerable interest in the past, because of a huge number of physical, chemical, and biological problems that can be described in terms of these equations [1–7]. Equation (1) is the simplest reaction-diffusion equation combining both the linear diffusion transport process and nonlinear chemical kinetics and admitting a traveling wave solution of the form $\rho(t,z) = \psi(t-uz)$. The basic advantage of the KPP equation is that the speed of traveling wave u can be found *exactly* in terms of the diffusion coefficient D and the growth rate constant U, namely, $u = \sqrt{4UD}$ (so-called minimal speed of propagation). However, from a physical point of view, the KPP equation has one disadvantage that can be explained as follows. It is easy to see from Eq. (1) that the kinetic term $U\rho(1-\rho)$ ensures that the maximal growth rate of the scalar field ρ occurs at those regions in the space where ρ is nearly zero. At the same time the diffusion approximation for transport processes is a very poor one for those regions. This is due to the fact that the ordinary diffusion term $D\partial^2\rho/\partial z^2$ gives rise to the infinite speed of heat/mass propagation: $\rho(t,z)$ is nonzero at any time $t \neq 0$ no matter how large z becomes. This might lead to an overestimation of the minimal speed of wave propagation, especially when the chemical kinetics constant U is relatively large. One way to overcome this problem is to modify the KPP kinetics introducing the preheated zone ahead of the reaction front where the chemical reaction is negligible [8]. Another way is to modify the transport process based on the diffusion approximation taking into account the finite speed of heat/mass propagation [9–12]. A quite different approach is based on the lattice-gas models for which the KPP equation can be viewed as the mean-field approximation [13,14] (see the review [15]). One

can also study the Langevin equations associated with the KPP equation (1) to analyze deviations from deterministic behavior [16,17].

In this paper we present a mean-field theory for the reaction-diffusion system involving diffusion with a finite speed and KPP kinetics. Recently [12] we introduced a probabilistic technique for analyzing reaction front dynamics for a one-dimensional reaction-diffusion system. By using a scaling procedure and functional integral technique together with large deviation theory for the Poisson random walk we have derived the exact formula for the reaction front speed. One of the motivations for the present study is to reinterpret this probabilistic method in terms of the nonlinear partial differential equation (PDE)-technique based on Hamilton-Jacobi type equations [18–21]. This interpretation allows us to extend the previous method to the n-dimensional case involving nonuniform space distribution of the chemical rate function, and offers a powerful way of finding the position of a reaction front and its speed of propagation.

II. FORMULATION OF THE PROBLEM

We consider a scalar field $\rho(t,\mathbf{r})$ (temperature, concentration, etc.) whose dynamics is governed by the transport equation with a reaction rate term of the KPP type,

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} = U(\varepsilon\mathbf{r})\rho(1-\rho), \quad \mathbf{r} \in R^n \tag{2}$$

where the reaction rate $U(\varepsilon\mathbf{r})$ is a slowly varying function of the space coordinate; ε is a small parameter which plays a very important role in what follows; $\mathbf{r} = (x_1, x_2, \ldots, x_n)$.

To take into account the finite speed of the transport process we assume that the heat/mass flux $\mathbf{J}$ is determined as an integral over time of the temperature/concentration gradient multiplied by the flux kernel $R(t-s)$ [10],

$$\mathbf{J}(t,\mathbf{r}) = -D \int_0^t R(t-s)\boldsymbol{\nabla}\rho(s,\mathbf{r})ds. \tag{3}$$

In this paper we choose an exponential kernel with a single relaxation time τ,

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$$R(t-s) = \frac{1}{\tau}\exp\left(\frac{t-s}{\tau}\right). \tag{4}$$

If $\tau = 0$, the system (2)–(4) reduces to the classical KPP equation

$$\frac{\partial \rho}{\partial t} = D\Delta\rho + U(\varepsilon\mathbf{r})\rho(1-\rho). \tag{5}$$

If $U = 0$, then we have the telegraph equation [9–11]

$$\tau\frac{\partial^2 \rho}{\partial t^2} + \frac{\partial \rho}{\partial t} = D\Delta\rho, \tag{6}$$

which describes a heat/mass transport by waves with a finite speed $v = \sqrt{D/\tau}$. The small value of τ explains the fact that in practice the diffusion approximation for the transport process appears to be sufficiently accurate in typical cases.

To summarize, we have the equation

$$\frac{\partial \rho}{\partial t} = \frac{D}{\tau}\int_0^t \exp\left(\frac{t-s}{\tau}\right)\Delta\rho(s,\mathbf{r})ds$$
$$+ U(\varepsilon\mathbf{r})\rho(1-\rho), \quad \mathbf{r}\in R^n \tag{7}$$

with the initial condition

$$\rho(0,\mathbf{r}) = \psi_0(\varepsilon\mathbf{r}), \tag{8}$$

where the initial function $\psi_0(\mathbf{r})$ has bounded support

$$\Omega_0 = \{\mathbf{r}\in R^n: \ \psi_0(\mathbf{r}) = 1\}. \tag{9}$$

In particular, the support might have a form of the ball such that

$$\rho(0,\mathbf{r}) = \begin{cases} 1 & \text{if } \sum_{i=1}^{n}\varepsilon^2 x_i^2 \leqslant R^2, \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

It follows from here that the small parameter ε can be considered as a measure of ratio between the characteristic front thickness $\sqrt{D/U}$ and characteristic length scale of the support of initial distribution.

Our purpose is to study the behavior of solutions of Eqs. (7)–(9) for large times of order ε^{-1} and find out whether or not there exists a traveling wave solution to Eqs. (7)–(9) in the limit $t\to\infty(\varepsilon\to 0)$. In this paper we will follow Freidlin's idea [6,7] that if a reaction-diffusion system possesses one unstable and one stable equilibrium, then, after appropriate rescaling in the space and time variables, the solution of the reaction-diffusion system converges to the indicator function of the set whose boundary may be considered as a moving wave front separating the stable and unstable regions.

We expect that after the hyperbolic scaling $t\to t/\varepsilon$, $\mathbf{r}\to\mathbf{r}/\varepsilon$ the new scalar field

$$\rho^\varepsilon(t,\mathbf{r}) = \rho\left(\frac{t}{\varepsilon},\frac{\mathbf{r}}{\varepsilon}\right) \tag{11}$$

takes only two values 0 and 1 as $\varepsilon\to 0$. The problem now is to derive the equation governing the geometrical evolution of

the reaction front separating the region where $\rho^\varepsilon(t,\mathbf{r})\to 0$ and the region where $\rho^\varepsilon(t,\mathbf{r})\to 1$.

III. REACTION FRONT EQUATION

Now we present a heuristic derivation of the equation governing the evolution of the reaction front. By using Eqs. (7)–(9) we can write down the equation for $\rho^\varepsilon(t,\mathbf{r})$:

$$\frac{\partial \rho^\varepsilon}{\partial t} = \frac{D}{\tau}\int_0^t \exp\left(-\frac{t-s}{\varepsilon\tau}\right)\Delta\rho^\varepsilon(s,\mathbf{r})ds$$
$$+ \frac{U(\mathbf{r})}{\varepsilon}\rho^\varepsilon(1-\rho^\varepsilon), \quad \mathbf{r}\in R^n \tag{12}$$

and the initial condition

$$\rho^\varepsilon(0,\mathbf{r}) = \psi_0(\mathbf{r}).$$

It is easy to see from Eq. (12) that in the limit $\varepsilon\to 0$ the reaction rate is very fast and the transport process is very slow and therefore the solution ρ^ε at each point, where $\rho^\varepsilon \neq 0$, tends quickly to the stable equilibrium value $\rho^\varepsilon = 1$. The set

$$\Omega_t = \{\mathbf{r}\in R^n: \ \lim_{\varepsilon\to 0}\rho^\varepsilon(t,\mathbf{r}) = 1\} \tag{13}$$

propagates throughout the region where $\rho^\varepsilon\to 0$ as $\varepsilon\to 0$ and our basic purpose is to find the location of the reaction front (the boundary of the set Ω_t) and the rate at which it moves.

Taking into account that Eqs. (3) and (4) are equivalent to

$$\frac{\partial \mathbf{J}}{\partial t} = -\frac{1}{\tau}\mathbf{J} - \frac{D}{\tau}\boldsymbol{\nabla}\rho, \quad \mathbf{J}(0,\mathbf{r}) = 0,$$

we can rewrite Eq. (12) in the form

$$\varepsilon\tau\frac{\partial^2 \rho^\varepsilon}{\partial t^2} + [1 - \tau U(\mathbf{r}) + 2\tau U(\mathbf{r})\rho^\varepsilon]\frac{\partial \rho^\varepsilon}{\partial t}$$
$$= \varepsilon D\Delta\rho^\varepsilon + \frac{U(\mathbf{r})}{\varepsilon}\rho^\varepsilon(1-\rho^\varepsilon). \tag{14}$$

Since $\rho^\varepsilon(t,\mathbf{r})\geqslant 0$ we can make an exponential transformation

$$\rho^\varepsilon(t,\mathbf{r}) = \exp\left(-\frac{G^\varepsilon(t,\mathbf{r})}{\varepsilon}\right), \quad G^\varepsilon(t,\mathbf{r})\geqslant 0. \tag{15}$$

This transformation has proved to be very useful in studying asymptotic problems for reaction-diffusion equations (see, for example, [19,20]). The new function $G^\varepsilon(t,\mathbf{r})$ will determine the location of the reaction front in the limit $\varepsilon\to 0$.

Straightforward calculation shows that $G^\varepsilon(t,\mathbf{r})$ satisfies the nonlinear PDE

$$-\tau\left(\frac{\partial G^{\varepsilon}}{\partial t}\right)^2+[1-\tau U(\mathbf{r})]\frac{\partial G^{\varepsilon}}{\partial t}+D(\boldsymbol{\nabla}G^{\varepsilon})^2+U(\mathbf{r})$$

$$=-\varepsilon\tau\frac{\partial^2 G^{\varepsilon}}{\partial t^2}+\varepsilon D\Delta G^{\varepsilon}+U(\mathbf{r})\left(1-2\tau\frac{\partial G^{\varepsilon}}{\partial t}\right)$$

$$\times\exp\left(-\frac{G^{\varepsilon}}{\varepsilon}\right).\tag{16}$$

Since $\exp(-G^{\varepsilon}/\varepsilon)\to 0$ as $\varepsilon\to 0$ for $G^{\varepsilon}>0$ we may conclude from Eq. (16) that the limiting function

$$G(t,\mathbf{r})=\lim_{\epsilon\to 0}G^{\varepsilon}(t,\mathbf{r})\tag{17}$$

obeys the nonlinear PDE of the first order,

$$-\tau\left(\frac{\partial G}{\partial t}\right)^2+[1-\tau U(\mathbf{r})]\frac{\partial G}{\partial t}+D(\boldsymbol{\nabla}G)^2+U(\mathbf{r})=0$$

$$[G(t,\mathbf{r})>0].\tag{18}$$

The advantage of the exponential transformation (15) is now apparent: Eq. (18) allows us to consider the problem of wave propagation for the reaction-diffusion system (12) in the geometric optic approximation [6,7,19,20]. The location of the reaction front can be determined as the boundary of the set

$$S=\{\mathbf{r}\in R^n:\ G(t,\mathbf{r})>0\}.\tag{19}$$

It is clear from Eq. (15) that $\rho^{\varepsilon}(t,\mathbf{r})\to 0$ as $\varepsilon\to 0$ for $\mathbf{r}\in S$. The fact that the boundary of the set S coincides with that of Ω_t [see Eq. (13)] has to be proved. It is easy to see that Eq. (18) goes over into the classical Hamilton-Jacobi equation in the limit $\tau\to 0$,

$$\frac{\partial G}{\partial t}+D(\boldsymbol{\nabla}G)^2+U(\mathbf{r})=0,$$

which is a basic tool for determining the reaction front dynamics for the classical KPP equation [17,19,20].

IV. RELATIVISTIC HAMILTON-JACOBI EQUATION

This section concerns the derivation of the explicit representation formula for $G(t,\mathbf{r})$. The basis idea is that Eq. (18) is identical in form to an equation arising in classical relativity theory. If we introduce new parameters

$$\varphi(\mathbf{r})=\frac{1}{2}\left[U(\mathbf{r})-\frac{1}{\tau}\right],\quad m(\mathbf{r})=\frac{\tau}{2D}\left[U(\mathbf{r})+\frac{1}{\tau}\right],\quad c^2=\frac{D}{\tau}$$
$$\tag{20}$$

then Eq. (18) can be rewritten in the form of the relativistic Hamilton-Jacobi equation for a particle with a mass m moving in the potential field $\varphi(\mathbf{r})$ [22],

$$\left(\frac{\partial G}{\partial t}+\varphi(\mathbf{r})\right)^2-m^2(\mathbf{r})c^4-c^2(\boldsymbol{\nabla}G)^2=0,\quad \mathbf{r}\in R^n$$

where c is the speed of light. It is interesting to note that the ''mass'' $m(\mathbf{r})$ depends on the space coordinate $\mathbf{r}$ [see Eq. (20)].

The Hamiltonian associated with this equation is

$$H(\mathbf{r},\mathbf{p})=\sqrt{m^2(\mathbf{r})c^4+c^2p^2}+\varphi(\mathbf{r}).\tag{21}$$

Since $\partial G/\partial t=-H$ Eq. (18) can be rewritten as

$$\frac{\partial G}{\partial t}+\sqrt{m^2(\mathbf{r})c^4+c^2(\boldsymbol{\nabla}G)^2}+\varphi(\mathbf{r})=0\tag{22}$$

or

$$\frac{\partial G}{\partial t}+\sqrt{\frac{1}{4}\left(U(\mathbf{r})+\frac{1}{\tau}\right)^2+\frac{D}{\tau}(\boldsymbol{\nabla}G)^2}+\frac{1}{2}\left(U(\mathbf{r})-\frac{1}{\tau}\right)=0.\tag{23}$$

The advantage of such an analogy is that we can write down the solution of Eq. (18) or Eq. (22) as

$$G(t,\mathbf{r})=\inf\left\{\int_0^t L\,ds:\ \mathbf{r}(0)=\mathbf{r},\ \mathbf{r}(t)\in\Omega_0\right\},\tag{24}$$

where the Lagrangian L has the form [22]

$$L=-m(\mathbf{r})c^2\sqrt{1-\frac{1}{c^2}\left(\frac{d\mathbf{r}}{ds}\right)^2}-\varphi(\mathbf{r}).\tag{25}$$

That is, the function $G(t,\mathbf{r})$ determining the reaction front position [see Eq. (19)] can be computed as the minimum over trajectories from $\mathbf{r}(0)=\mathbf{r}$ to $\mathbf{r}(t)\in\Omega_0$. The optimal trajectories satisfy the Euler-Lagrange equation

$$\frac{d}{ds}\left(\frac{\partial L}{\partial\dot{\mathbf{r}}}\right)-\frac{\partial L}{\partial\mathbf{r}}=0.\tag{26}$$

Using the relations (20), we find an expression for the Lagrangian L in terms of the phenomenological parameters τ, D, and $U(\mathbf{r})$,

$$L=-\frac{1}{2}\left(U(\mathbf{r})+\frac{1}{\tau}\right)\sqrt{1-\frac{\tau}{D}\left(\frac{d\mathbf{r}}{ds}\right)^2}-\frac{1}{2}\left(U(\mathbf{r})-\frac{1}{\tau}\right).$$

Thus, the analogy with the relativistic mechanics allows us to derive the explicit expression for the function $G(t,\mathbf{r})$ and thereby to find the reaction front position and its speed. It is clear that the calculation of $G(t,\mathbf{r})$ is greatly simplified when the reaction rate constant $U(\mathbf{r})$ does not depend on the space coordinate $\mathbf{r}$ (see next section).

V. EXACT FORMULA FOR A WAVE-FRONT PROPAGATION RATE

We now consider the case of a constant value of the chemical rate function U for which the action functional G can be calculated exactly. This will allow us to find explicit expressions for the position of reaction front and the speed of propagation.

When $U=$ const, the optimal trajectory is that of a free particle, i.e., the straight line connecting the points $\mathbf{r}$ and $\mathbf{y}\in\Omega_0$,

$$\mathbf{r}(s) = \left(\frac{\mathbf{y}-\mathbf{r}}{t}\right)s + \mathbf{r}, \quad 0 \leq s \leq t. \tag{27}$$

After substituting Eq. (27) into Eqs. (24) and (25) the action integral (24) can be written as

$$G(t,\mathbf{r}) = \inf_{\mathbf{y} \in \Omega_0} \left\{ -mc^2 t \sqrt{1 - \frac{1}{c^2}\left(\frac{\mathbf{y}-\mathbf{r}}{t}\right)^2} - \varphi t \right\}. \tag{28}$$

Let us denote by $l(\mathbf{r}, \Omega_0)$ the minimal distance between the point $\mathbf{r}$ and the set Ω_0. Then, in terms of the phenomenological parameters τ, D, and U, the action functional $G(t,\mathbf{r})$ can be rewritten as

$$G(t,\mathbf{r}) = -\frac{t}{2}\left(U + \frac{1}{\tau}\right)\sqrt{1 - \frac{\tau}{D}\left(\frac{l(\mathbf{r},\Omega_0)}{t}\right)^2} + \frac{t}{2}\left(\frac{1}{\tau} - U\right). \tag{29}$$

Now we are in a position to determine the exact formula for the reaction front propagation rate. It follows from Eq. (26) that the set $S = \{\mathbf{r} \in R^n : G(t,\mathbf{r}) > 0\}$ where $\rho^\varepsilon(t,\mathbf{r}) \to 0$ as $\varepsilon \to 0$ can be represented as

$$S = \{\mathbf{r} \in R^n : \ l(\mathbf{r}, \Omega_0) > ut\},$$

where

$$u = c\sqrt{1 - \left(\frac{1-\tau U}{1+\tau U}\right)^2} = \frac{\sqrt{4DU}}{1+\tau U}, \quad \tau U \leq 1. \tag{30}$$

It is clear that the velocity u can be considered as the propagation rate of the wave front. It follows from Eq. (30) that the effect of diffusion with finite velocity ($\tau U \neq 0$) is to decrease the propagation rate corresponding to the classical KPP equation. The last restriction $\tau U \leq 1$ comes from the fact that the ''speed of light'' $c = \sqrt{D/\tau}$ is the maximal velocity of heat/mass propagation. In other words, wave-front motion with greater velocity than the ''speed of light'' c is impossible.

If the support of the initial distribution has a form of the ball with the radius R,

$$\Omega_0 = \left\{ \sum_{i=1}^n x_i^2 \leq R^2 : \ \psi = 1 \right\}, \tag{31}$$

then the action functional G depends only on $r = \sqrt{\sum_{i=1}^n x_i^2}$ and t,

$$G(t,r) = -mc^2 t \sqrt{1 - \frac{1}{c^2}\left(\frac{R-r}{t}\right)^2} - \varphi t. \tag{32}$$

By equating $G(t,r)$ to zero, we find the exact formula for the position of the wave front $r(t)$,

$$r(t) = R + ut, \tag{33}$$

with u determined by Eq. (30).

We may call the line $r(t) = R + ct$ with $c = \sqrt{D/\tau}$ the primary wave front, referring to the fact that $\rho^\varepsilon(t,r) = 0$ for $r > R + ct$. In general, the formula for the propagation speed u can be written as

$$u = \begin{cases} \dfrac{\sqrt{4DU}}{1+\tau U} & \text{if } \tau U \leq 1, \\[3mm] \sqrt{\dfrac{D}{\tau}} & \text{if } \tau U > 1. \end{cases}$$

In the limiting case when the relaxation time τ is small compared with the chemical time U^{-1}, that is, $\tau U \ll 1$, we can neglect the effect of finiteness of the velocity of heat propagation.

VI. SUMMARY

In this paper we have analyzed the n-dimensional reaction-diffusion system involving diffusion with finite velocity and Kolmogorov-Petrovskii-Piskunov kinetics. By using hyperbolic scaling and nonlinear PDE techniques we have derived an equation governing the reaction front dynamics in the long-time large-distance limit. We have shown that the resulting equation is identical to the relativistic Hamilton-Jacobi equation for a particle moving in a potential field. In the case of a constant value of chemical rate we have derived the exact formula for the speed of reaction front and shown that the wave front propagates slower than that of the classical KPP equation.

It should be noted that there are several possible directions to investigate. First, one may formulate the whole problem in terms of variational inequality [19,20] and give the rigorous proofs for the results presented in this paper. Also, it would be interesting to apply the method developed here to the analyses of turbulent burning velocity [23–25].

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