BRIEF REPORTS

Brief Reports are accounts of completed research which do not warrant regular articles or the priority handling given to Rapid Communications; however, the same standards of scientific quality apply. (Addenda are included in Brief Reports.) A Brief Report may be no longer than four printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

Traveling waves in a reaction-diffusion system: Diffusion with finite velocity and Kolmogorov-Petrovskii-Piskunov kinetics

Sergei Fedotov*
Department of Mathematics, UMIST (University of Manchester Institute of Science and Technology), Manchester M60 1QD, United Kingdom
and Potsdam Institute for Climate Impact Research (PIK), Telegrafenberg C4, Potsdam 14412, Germany
(Received 1 May 1998)

An asymptotic method is presented for the analysis of the traveling waves in the one-dimensional reaction-diffusion system with the diffusion with a finite velocity and Kolmogorov-Petrovskii-Piskunov kinetics. The analysis makes use of the path-integral approach, scaling procedure, and the singular perturbation techniques involving the large deviations theory for the Poisson random walk. The exact formula for the position and speed of reaction front is derived. It is found that the reaction front dynamics is formally associated with the relativistic Hamiltonian/Lagrangian mechanics. [S1063-651X(98)14710-4]

PACS number(s): 82.20.Db, 05.70.Ln, 05.60.+w

Phenomena of the wave propagation in nonequilibrium media described by reaction-diffusion equations have attracted considerable interest in a wide variety of scientific fields including physics, chemistry, biology, etc. Excellent reviews of the work in this area can be found in the books [1–4]. Of fundamental interest is the rate at which the wave propagates through the nonlinear dissipative system. The basic common feature in many examples is that the transport process determining the propagation rate is described by the conventional diffusion (Fick's law). In this case the propagation velocity u can be found from a simple dimensional analysis, that is, $u \sim \sqrt{DU}$, where D is the diffusion coefficient and U is the characteristic reaction rate constant.

It is well known that the diffusion approximation gives rise to the infinite speed of heat/mass propagation, that is, if a sudden change of temperature/concentration takes place somewhere in the space, it will be felt immediately everywhere with an exponentially small amplitude. It is therefore desirable to have a theory for nonlinear wave propagation in which the boundness of the transport process would be taken into account. The purpose of this paper is to present such a theory giving an asymptotic method for calculating the propagation speed for the traveling wave in the reaction-diffusion system involving the diffusion with a finite velocity [5–10] and the chemical kinetics of Kolmogorov-Petrovskii-Piskunov (KPP) type [1–4,11–17].

Our starting point is a phenomenological system of the one-dimensional equations for the time evolution of the scalar field ρ and its flux J,

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

$$\frac{\partial J}{\partial t} = -\frac{J - J_0}{\tau}, \quad J_0 = -D\frac{\partial \rho}{\partial x}, \tag{2}$$

where U is the reaction rate constant corresponding to the KPP kinetics, D is the diffusion coefficient corresponding to Fick's law, and τ is the relaxation time. When $U=0$, the system (1),(2) reduces to the telegraph equation [5–10]

$$\tau\frac{\partial^2 \rho}{\partial t^2} + \frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2}. \tag{3}$$

When $\tau=0$, we have the classical KPP equation [1–4]

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} + U\rho(1-\rho). \tag{4}$$

If we now solve Eq. (2) with the initial condition $J(0,x)=0$ we may eliminate J from Eq. (1) to obtain the single equation for ρ,

$$\frac{\partial \rho}{\partial t} = \frac{D}{\tau}\int_0^t \exp\left(-\frac{t-s}{\tau}\right)\frac{\partial^2 \rho(s,x)}{\partial x^2}\,ds + U\rho(1-\rho). \tag{5}$$

This equation may be considered as a generalization of the KPP equation (4) to the case in which the finite speed of the transport process is taken into account ($\tau \neq 0$).

We specify the following initial condition:

$$\rho(0,x) = \theta(x), \tag{6}$$

*Electronic address: fedotov@pik-potsdam.de

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

The basic problem is to find the traveling wave solution $\psi(x-ut)$ to the problem (5),(6), where $\psi(z)$ is a monotonically decreasing function such that $\psi(-\infty)=1$ and $\psi(\infty)=0$, and u is the speed at which the wave profile ψ moves in the positive x direction. For the KPP equation (4) ($\tau=0$) with the initial condition (6) the traveling wave moves with the velocity $u=\sqrt{4DU}$ [1–4]. We expect that for Eqs. (5) and (6) the speed $u=\sqrt{4DU}f(\tau U)$, where $f(z)$ is the dimensionless function such that $f(0)=1$. It should be noted that our method of calculation will be nonperturbative in the sense that we do not treat the relaxation time τ as a small parameter.

We are interested in the long-time large-distance behavior of the traveling wave solution of Eqs. (5) and (6) as $t\to\infty$ and $x\to\infty$. It is convenient therefore to make the scaling [12–17]

$$t\to\frac{t}{\varepsilon},\quad x\to\frac{x}{\varepsilon}, \tag{7}$$

where ε is a small parameter, and rewrite the Cauchy problem (5),(6) for $\rho^{\varepsilon}(t,x)=\rho(t/\varepsilon\,,x/\varepsilon)$ in the following form:

$$\frac{\partial\rho^{\varepsilon}}{\partial t}=\frac{D}{\tau}\int_0^t\exp\left(-\frac{t-s}{\varepsilon\tau}\right)\frac{\partial^2\rho^{\varepsilon}(s,x)}{\partial x^2}ds + \frac{U}{\varepsilon}\rho^{\varepsilon}(1-\rho^{\varepsilon}),\quad \rho^{\varepsilon}(0,x)=\theta(x). \tag{8}$$

It is clear from this equation that the scaling (7) describing a simultaneous contraction of time and space alternatively corresponds to the rapid chemical reaction and slow transport process. We expect that after rescaling the wave profile develops into the reaction front: $\rho^{\varepsilon}(t,x)=\psi[(x-ut)/\varepsilon)]$ tends to a unit step function $\theta(x-ut)$ as $\varepsilon\to0$.

Our goal is now to find a function $G(t,x)$ determining the position of the reaction front, that is,

$$\lim_{\epsilon\to0}\rho^{\varepsilon}(t,x)=\begin{cases}0 & \text{if } G(t,x)<0\\ 1 & \text{otherwise.}\end{cases} \tag{9}$$

In this paper we restrict ourselves to finding the upper bound for $\rho^{\varepsilon}(t,x)$ in the form

$$\rho^{\varepsilon}(t,x)\leqslant\exp\left\{\frac{G(t,x)}{\varepsilon}\right\}\quad\text{as}\quad\varepsilon\to0. \tag{10}$$

Since $\rho^{\varepsilon}(t,x)$ varies in the interval $[0,1]$ it is clear from Eq. (10) that $\rho^{\varepsilon}(t,x)\to0$ if $G(t,x)<0$, $\varepsilon\to0$.

It follows from the property of the KPP kinetics in Eq. (8) that

$$\rho^{\varepsilon}(t,x)\leqslant\varphi^{\varepsilon}(t,x)\exp\left(\frac{Ut}{\varepsilon}\right), \tag{11}$$

where $\varphi^{\varepsilon}(t,x)$ is a solution of the linear initial problem

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

$$\varphi^{\varepsilon}(0,x)=\theta(x). \tag{12}$$

Our strategy to find the function $G(t,x)$ is to analyze the above Cauchy problem in terms of the probability theory and thereby to obtain an estimate of $\varphi^{\varepsilon}(t,x)$ in the limit $\varepsilon\to0$. The basic idea is that we can deal with the problem (12) in terms of the random walks of Poisson type [7–9]. If we introduce the notations c (velocity) and ν (frequency) such that

$$c^2=\frac{D}{\tau},\quad 2\nu=U+\frac{1}{\tau}, \tag{13}$$

then the solution of linear initial value problem (12) can be written as an expectation value of the initial distribution θ [7,8],

$$\varphi^{\varepsilon}(t,x)=E\,\theta(x(t)), \tag{14}$$

where E is the expectation operator and $x(t)$ is a random Poisson walk, i.e., a solution of the stochastic differential equation

$$\frac{dx}{ds}=v\left(\frac{s}{\varepsilon}\right),\quad x(0)=x,\quad 0<s<t \tag{15}$$

where $v(s)$ is the Markovian dichotomous velocity taking only two values $\{c,-c\}$ with the frequency ν [18]. From the probabilistic point of view the key factor underlying the nonlocal character of Eq. (12) is that the dynamics of $x(t)$ is non-Markovian [18]. To obtain an estimate of $\varphi^{\varepsilon}(t,x)$ as $\varepsilon\to0$ we need to know an explicit expression for $\varphi^{\varepsilon}(t,x)$ as a path integral [19],

$$\varphi^{\varepsilon}(t,x)=\int\theta(x(t))P[x(\cdot)]\mathcal{D}x, \tag{16}$$

where $P[x(\cdot)]$ is a conditional probability density functional for the random process $x(s)$,

$$P[x(\cdot)]=\int\delta\left[\frac{dx}{ds}-v\left(\frac{s}{\varepsilon}\right)\right]P[v(\cdot)]\mathcal{D}v,$$

where $\delta[\cdot]$ is the δ functional that is the extension of the ordinary δ function to the functional integration [19]. By using Eq. (16) and the formalism based on the auxiliary function u [20,21] we can write down the following expression for $\varphi^{\varepsilon}(t,x)$:

$$\varphi^{\varepsilon}(t,x)=\int\int\int\theta(x(t))\exp\left\{i\int_0^t u(s)\left[\frac{dx}{ds}-v\left(\frac{s}{\varepsilon}\right)\right]ds\right\}\times P[v(\cdot)]\mathcal{D}v\,\mathcal{D}u\,\mathcal{D}x. \tag{17}$$

In the ''weak noise limit'' $\varepsilon\to0$ one can get the following estimate for $\varphi^{\varepsilon}(t,x)$ (the details of calculation involving the large deviations theory for the Poisson random walk will appear elsewhere):

$$\varphi^{\varepsilon}(t,x)\sim\exp\left\{-\frac{1}{\varepsilon}\min_{x(0)=x;x(t)=0}\int_0^t\left(p\frac{dx}{ds}-H(p)\right)ds\right\}, \tag{18}$$

where the function $H(p)$ has the form of the relativistic Hamiltonian [22]

$$H(p)=c\sqrt{m^2c^2+p^2}-\nu, \tag{19}$$

with the ''effective mass'' $m=\nu c^{-2}$. One can rewrite Eq. (18) in terms of the relativistic Lagrangian [22]

$$\varphi^{\varepsilon}(t,x)\sim\exp\left\{-\frac{1}{\varepsilon}\min_{x(0)=x;x(t)=0}\int_0^t L\,ds\right\}, \tag{20}$$

where

$$L=-mc^2\sqrt{1-\frac{1}{c^2}\left(\frac{dx}{ds}\right)^2}+\nu. \tag{21}$$

We are now in a position to complete the derivation of the function $G(t,x)$ determining the reaction front position and its speed. One finds after straightforward calculation that the optimal trajectory giving the minimum in Eq. (20) is $x(s)=-(x/t)s+x$ and the corresponding minimal action is $-mc^2t\sqrt{1-(1/c^2)(x/t)^2}+\nu t$. By using Eqs. (10), (11), and (20) and the relation $m=\nu c^{-2}$ we obtain

$$G(t,x)=Ut-\nu t+\nu t\sqrt{1-\frac{1}{c^2}\left(\frac{x}{t}\right)^2}. \tag{22}$$

Equating $G(t,x)$ to 0 we obtain the position of reaction front $x(t)$,

$$x(t)=ut,\quad u=c\sqrt{1-\left(\frac{\nu-U}{\nu}\right)^2},\quad U\leqslant\nu. \tag{23}$$

Taking into account Eq. (13) the speed of the reaction front u can be rewritten in terms of the phenomenological parameters D and τ,

$$u=\frac{\sqrt{4DU}}{1+\tau U},\quad \tau U\leqslant 1. \tag{24}$$

We suggest that $u=\sqrt{D/\tau}$ when $\tau U>1$. It follows from Eqs. (23) and (24) that the speed u takes the maximum value $c=\sqrt{D/\tau}$, when $\tau U=1$ or $U=\nu$. If the velocity of propagation c were infinitely great and the time τ were infinitely small such that $D=c^2\tau=\text{const}$ (the diffusion approximation for the random walk of Poisson type), Eq. (23) would merely give $u=\sqrt{4DU}$—the classical result of the KPP theory [1–4].

In summary, we have derived the *exact* formula for the position and speed of the reaction front in the one-dimensional dissipative system involving the diffusion with a finite velocity and the KPP kinetics. It has been found that the reaction front dynamics for such a system can be formally associated with the relativistic Hamiltonian/Lagrangian mechanics. There are several possible directions to explore by the method developed here. First one may study the influence of nonuniform distribution of the reaction rate constant U which might induce the jumps of reaction fronts [11]. One can also extend the analysis to describe the interaction between the turbulent diffusion with a finite velocity [10] and the KPP kinetics in the three-dimensional space [17].

The author would like to thank Rupert Klein and Alexander S. Mikhailov for interesting and helpful discussions. The research was supported in part by DFG Project No. KL 611/5-1.

[1] N. F. Britton, *Reaction-Diffusion Equations and Their Applications to Biology* (Academic Press, New York, 1986).
[2] V. A. Vasilev, Zu. M. Romanovskii, D. S. Chernavskii, and V. G. Yakhno, *Autowave Processes in Kinetic Systems* (Reidel, Dordrecht, 1986).
[3] J. D. Murray, *Mathematical Biology* (Springer, Berlin, 1989).
[4] A. S. Mikhailov, *Foundations of Synergetics I: Distributed Active Systems* (Springer-Verlag, Berlin, 1990).
[5] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics I* (McGraw-Hill, New York, 1953).
[6] D. D. Joseph and L. Preziosi, Rev. Mod. Phys. **61**, 41 (1989).
[7] S. Goldstein, Q. J. Mech. Appl. Math. **4**, 129 (1951).
[8] C. DeWitt-Morette and S. K. Foong, Phys. Rev. Lett. **62**, 2201 (1989).
[9] S. K. Foong and U. van Kolck, Prog. Theor. Phys. **87**, 285 (1992).
[10] A. Monin and A. Yaglom, *Statistical Fluid Mechanics* (MIT Press, Cambridge, MA, 1987).
[11] M. Freidlin, *Functional Integration and Partial Differential Equations* (Princeton University Press, Princeton, NJ, 1985).
[12] M. Freidlin, in *Semi-linear PDE's and Limit Theorems for Large Deviations*, edited by P. L. Hennequin, Lecture Notes in Mathematics Vol. 1527 (Springer, Berlin, 1992).
[13] P. Souganidis and A. Majda, Nonlinearity **7**, 1 (1994).
[14] P. Souganidis and A. Majda, J. Stat. Phys. **83**, 933 (1996).
[15] S. Fedotov, Phys. Rev. E **52**, 3835 (1995).
[16] S. Fedotov, J. Phys. A **29**, L517 (1996).
[17] S. Fedotov, Phys. Rev. E **55**, 2750 (1997).
[18] *Noise in Nonlinear Dynamical Systems*, edited by F. Moss and P. V. E. McClintock (Cambridge University Press, Cambridge, England, 1989), Vols. I and II.
[19] F. Langouche, D. Roekaerts, and E. Tirapegui, *Functional Integration and Semiclassical Expansions* (Reidel, Dordrecht, 1982).
[20] H. K. Janssen, Z. Phys. B **23**, 377 (1976).
[21] R. Graham and T. Tel, Phys. Rev. A **31**, 1109 (1986).
[22] L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields* (Pergamon, Oxford, 1960).