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LETTER TO THE EDITOR

Travelling kinks collision in Schlögl's second model for non-equilibrium phase transitions

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Abstract. It is shown how to obtain an exact solution class of the nonlinear reaction diffusion equation in Schlögl's second model. For large time these solutions evolve to bounded travelling kinks. When the phase coexistence conditions are satisfied, the solutions describe the collision of two travelling kinks.

The considered system represents an autocatalytic chemical reaction model and was introduced by Schlögl (1972) as an example for a non-equilibrium phase transition. The system of reactions occurring in both directions is given by

$$A+2X \leftrightarrows 3X \tag{1}$$

$$B+X \leftrightarrows C \tag{2}$$

where the concentrations a, b, c of the species A, B, C are held constant in space and time by adequate external feeding. For the species X the system is assumed to be closed, so that the time behaviour of the concentration n from the species X will be determined only by the dynamics of equations (1) and (2).

There can exist two stable and one unstable steady states with homogeneous n. In analogy with a gas–fluid system the two stable states can be interpreted as two phases (Schlögl 1972).

When diffusion of X in one direction z is included, the two spatially separated phases can coexist in the reaction system. By choosing appropriate units of time, length and concentration, the variable concentration n fulfils the semilinear parabolic equation

$$\partial n/\partial t - D\partial^2 n/\partial z^2 = \varphi(n) \tag{3}$$

with the kinetic rate function

$$\varphi(n) = -n^3 + 3\alpha n^2 - \beta n + \gamma \tag{4}$$

where D is a diffusion constant and α, β, γ are positive real control parameters related respectively to the concentrations of the species A, B and C. The factor 3 is introduced for convenience.

This reaction diffusion system was studied by various authors in deterministic theory (Schlögl 1972, Schlögl and Berry 1980, Ebeling 1976, Ebeling and Malchow 1979, Dung and Kozak 1981, Magyari 1982). Over the last few years semilinear parabolic equations of the general form of (3) have attracted mathematical interest since they occur in a wide field of natural sciences (Fisher 1930, 1937, Gelfand 1959, 1963, Livshits *et al* 1981). Some authors have studied the existence and convergence of travelling wave fronts by mathematical analysis (Fife 1977, 1979, Fife and McLeod 1977, 1981, Rothe 1978, Hallam 1979, Uchiyama 1978, Paulwelussen 1981, Donnelly 1980, Sperb 1981).

The following procedure is not restricted to the Schlögl model with positive real quantities n, α, β, γ because of the connection with chemical reactions. When β is below a critical value $\beta_c = 3\alpha^2$ there exist three homogeneous steady states of (3) and $\varphi(n)$ can be expressed as

$$\varphi(n) = -(n-n_1)(n-n_2)(n-n_3)$$

where $n_2 \leqslant n_3 \leqslant n_1$ are the real roots of $\varphi(n)=0$. For the following, it will be convenient to transform equations (3) and (4) by the substitutions (Schlögl and Berry 1980)

$$\nu(z,t) = n(z,t) - \bar{n} \qquad \bar{n} = \tfrac{1}{2}(n_1+n_2) \qquad \nu_0 = \tfrac{1}{2}(n_2 - n_1) \qquad n_3 = \bar{n} + \nu_0 a$$

where a is a real constant with $-1 \leqslant a \leqslant +1$. The transformed equation (3) can thus be written

$$\partial\nu/\partial t - D\partial^2\nu/\partial z^2 = -(\nu - \nu_0 a)(\nu^2 - \nu_0^2) = \varphi(\nu). \tag{5}$$

When $a=0$, the phase coexistence conditions are satisfied and the two stable homogeneous steady states ν^* are $\nu_1^* = +\nu_0$ and $\nu_2^* = -\nu_0$. The unstable state is $\nu_3^* = 0$. In analogy with a gas–fluid system these conditions are fulfilled by a special value for the control parameter γ in (4) obtained by the Maxwellian construction (Schlögl 1972) where the reaction rate function satisfies

$$\int_{n_1}^{n_2} \mathrm{d}n\, \varphi(n) = 0. \tag{6}$$

When $a \neq 0$, the integral (6) is not vanishing and γ differs from the coexistence value. Now there exist only one stable and two unstable homogeneous steady states.

Travelling wave solutions from (5) were recently written down for $a \neq 0$ by Schlögl and Berry (1980) and for $a=0$ by Magyari (1982). Such solutions are of the form

$$\nu(z,t) = g(\eta) \tag{7}$$

where $\eta = pt + qz$ with real constants p and q. The substitution (7) transforms (5) into an ordinary differential equation for $g(\eta)$.

We are looking for more general solutions of (5) fulfilling the condition (7) only in the asymptotic case for large time t. For this purpose we introduce a continuous function $\mu(z,t)$ with continuous first derivative for z, so that we can define the following relation between $\nu(z,t)$ and $\mu(z,t)$:

$$\nu(z,t) = (2D)^{1/2}(1/\mu(z,t))\partial\mu(z,t)/\partial z. \tag{8}$$

The substitution (8) transforms (5) into the partial differential equation for $\mu(z,t)$

$$\mu\left(\frac{\partial^2\mu}{\partial z\,\partial t} - D\frac{\partial^3\mu}{\partial z^3} - \nu_0^2\frac{\partial\mu}{\partial z} + \nu_0^3 a(2D)^{-1/2}\mu\right) = \frac{\partial\mu}{\partial z}\left(\frac{\partial\mu}{\partial t} - 3D\frac{\partial^2\mu}{\partial z^2} + \nu_0 a(2D)^{+1/2}\frac{\partial\mu}{\partial z}\right). \tag{9}$$

Solutions from (9) can easily be gained when the expressions in the brackets vanish. Eliminating $\partial^2\mu/\partial z\,\partial t$ in the left-hand brackets by the derivation for z of the right-hand brackets, we find the linear system for $\mu(z, t)$

$$2D\partial^3\mu/\partial z^3 - \nu_0 a(2D)^{+1/2}\partial^2\mu/\partial z^2 - \nu_0^2\partial\mu/\partial z + \nu_0^3 a(2D)^{-1/2}\mu = 0 \quad (10)$$

$$\partial\mu/\partial t - 3D\partial^2\mu/\partial z^2 + \nu_0 a(2D)^{+1/2}\partial\mu/\partial z = 0. \quad (11)$$

Equation (10) can be solved as an ordinary differential equation with time-dependent integration constants since the time t can be considered as a parameter. The ansatz

$$\mu \sim \exp[r(2D)^{-1/2}z]$$

leads to the characteristic equation of (10) which has the form of the kinetic rate function $\varphi(r) = 0$ with the real roots $r_1 = +\nu_0$, $r_2 = -\nu_0$, $r_3 = a\nu_0$. The general solution of (10) can then be written as

$$\mu(z, t) = \hat{c}_1(t)\,\mathrm{e}^{\sigma z} + \hat{c}_2(t)\,\mathrm{e}^{-\sigma z} + \hat{c}_3(t)\,\mathrm{e}^{a\sigma z} \quad (12)$$

where $\sigma = \nu_0(2D)^{-1/2}$.

The time-dependent functions $\hat{c}_i(t)$ can now be determined by substituting (12) in (11), and we then obtain the general solution of the linear system (10), (11)

$$\mu(z, t) = (c_1 u + c_2 u^{-1} + c_3 v)\exp(\tfrac{3}{2}\nu_0^2 t)$$

where c_1, c_2, c_3 are real integration constants and u and v are abbreviations defined by

$$u = \exp(-\nu_0^2 a t + \sigma z) \qquad v = \exp[\tfrac{1}{2}\nu_0^2(a^2 - 3)t + a\sigma z].$$

With the relation (8), the solution of (5) yields finally

$$\nu(z, t) = \nu_0(c_1 u - c_2 u^{-1} + a c_3 v)/(c_1 u + c_2 u^{-1} + c_3 v). \quad (13)$$

The constants c_i define various solution classes of (5). The homogeneous steady ν^* are obtained when two of the constants vanish:

$$\nu^* = \nu_0 a \qquad \text{for } c_1 = c_2 = 0$$

$$\nu^* = -\nu_0 \qquad \text{for } c_1 = c_3 = 0$$

$$\nu^* = +\nu_0 \qquad \text{for } c_2 = c_3 = 0.$$

Travelling kinks $\tilde{\nu}$, $\nu^{(+)}$, $\nu^{(-)}$ are obtained when only one constant vanishes:

$$\tilde{\nu}(z, t) = \nu_0 \tanh(\sigma z - \nu_0^2 a t + z_0) \qquad \text{for } c_3 = 0 \quad (14)$$

and $\nu^{(+)}$ for $c_2 = 0$ and $\nu^{(-)}$ for $c_1 = 0$ where

$$\nu^{(\pm)} = \nu_0 a \pm \nu_0(1 \mp a)\{1 + \exp[\tfrac{1}{2}\nu_0^2(a \pm 3)(a \mp 1)t + \sigma(a \mp 1)z + z_0]\}^{-1}. \quad (15)$$

With non-vanishing constants c_i the solution (13) evolves for large time t to the travelling kinks $\tilde{\nu}(z, t)$ of (14). This is also valid in the coexistence case for $a = 0$. $\tilde{\nu}$ becomes the inhomogeneous stationary coexistence solution of (4). Then the initial value $\nu(z, t = 0)$ of (13) can be expressed as the sum of the initial values of $\nu^{(+)}$ and $\nu^{(-)}$ given by (15),

$$\nu(z, t = 0) = \nu^{(+)}(z, t = 0) + \nu^{(-)}(z, t = 0) \qquad (\text{for } a = 0),$$

so that the solution (13) describes the collision of the travelling kinks $\nu^{(+)}$ and $\nu^{(-)}$.

The aim in this work was to gain a more general solution than the travelling wave fronts in the reaction diffusion system of Schlögl's second model for a non-equilibrium phase transition. The substitution (8) transforms the parabolic equation with cubic nonlinearity into a form offering access to the searched-for solution. One can easily see that the same method is applicable for systems with spherical or cylindrical symmetry.

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