LETTER TO THE EDITOR

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

E Magyari

Institut für Physik der Universität Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Abstract. By using the separation technique recently developed by Osborne and Stuart, travelling wave solutions are written down for the nonlinear reaction–diffusion equation of Schlögl's second model, assuming that the necessary conditions for the static phase-coexistence are satisfied.

Ten years ago Schlögl devised two simple chemical reaction models (Schlögl 1972) which exhibit the behaviour of the first- and second-order non-equilibrium phase transitions, respectively. Schlögl's second model which exhibits first-order behaviour, including the coexistence of two spatially separated phases, is connected with the autocatalytic chemical reactions

$$A + 2X \underset{k_1'}{\overset{k_1}{\rightleftharpoons}} 3X, \qquad B + X \underset{k_2'}{\overset{k_2}{\rightleftharpoons}} C, \tag{1}$$
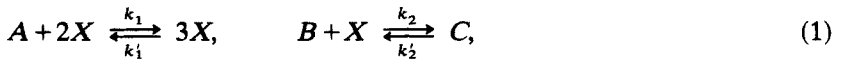
where the concentrations a, b, c of the species A, B, C and the reaction rates k_i, k_i' are externally kept fixed and only the concentration n of the intermediate product X can vary in time and space due to the chemical reactions and diffusion. Under these conditions, the evolution of n in Schlögl's second (one-dimensional) model with uniform diffusion (D = constant) is governed by the nonlinear parabolic equation (Schlögl 1972)

$$\partial n/\partial t - \partial^2 n/\partial z^2 = -n^3 + 3n^2 - \beta n + \gamma \tag{2}$$

where $\beta = 9k_1'k_2'b/k_1^2a^2$ and $\gamma = 27k_1'^2k_2'c/k_1^3a^3$ are positive parameters and $n = n(z, t) \geq 0$, $-\infty < t, z < +\infty$, are scaled dimensionless quantities (the corresponding physical quantities are measured in units of $\langle n \rangle = k_1a/3k_1'$, $\langle t \rangle = 9k_1'/k_1^2a^2$ and $\langle z \rangle = 3(Dk_1')^{1/2}/k_1a$, respectively). Regarding

$$\beta = \gamma + 2 \qquad \text{with} \quad 0 < \gamma < 1, \tag{3}$$

equation (2) admits the positive uniform ($\partial n/\partial t \equiv 0$, $\partial n/\partial z \equiv 0$) solutions

$$n_{1,2} = 1 \pm (1 - \gamma)^{1/2}, \qquad n_3 = 1, \tag{4}$$

where $n_{1,2}$ are stable and n_3 is unstable (Schlögl 1972). In static conditions ($\partial n/\partial t \equiv 0$), i.e. when the variation of n due to the chemical reactions is instantaneously balanced

in each elementary volume of the system by its variation due to the diffusion, the stable uniform solutions $n_{1,2}$ represent the concentrations of the species X in two coexistent but spatially separated phases, connected to each other by a thin kink $(+)$ or antikink $(-)$ shaped boundary layer (Schlögl 1972):

$$n_s(z) = 1 \pm (1-\gamma)^{1/2} \tanh \{[\tfrac{1}{2}(1-\gamma)]^{1/2} z\}. \tag{5}$$

Our aim in this Letter is to obtain travelling wave (TW) solutions to equation (2) by using the separation technique recently developed by Osborne and Stuart (Osborne and Stuart 1978, 1980a, b, Osborne 1981), assuming at the same time that the necessary conditions (3) of the static phase-coexistence are satisfied.

According to the Osborne–Stuart (OS) separation scheme, we are looking for the solution of equation (2) in the form of a dependent variable transformation

$$n(z, t) = g(\eta), \tag{6}$$

where η is a separable function of z and t. Choosing further $\eta = K \exp[r(z - ut)]$, where K, r and u are non-vanishing real constants, the existence of (separable) TW solutions is guaranteed for a large class of nonlinear evolution equations (Osborne 1981). In our case, taking into account also (3), equation (2) becomes

$$r^2\eta^2 g'' + r(r+u)\eta g' - g^3 + 3g^2 - (\gamma+2)g + \gamma = 0, \tag{7}$$

where the prime indicates $d/d\eta$. Further, let us substitute in equation (6)

$$g(\eta) = p + \eta^s y(\xi), \qquad \xi = \eta^q, \tag{8}$$

where p, q, s are constants, ξ is a new variable and y a new function. Now, by choosing $p = 1$, $s = q = 3(\gamma-1)/2ru$ and $u^2 = 9(1-\gamma)/2$, we obtain for y the equation $(1-\gamma)(d^2 y/d\xi^2) = 2y^3$, which yields the first integral

$$(1-\gamma)(dy/d\xi)^2 - y^4 = \text{constant}. \tag{9}$$

This equation may by the substitution $y = \pm(1-\gamma)^{1/2}\mathscr{P}^{1/2}(\xi + \xi_0, g_2, g_3)$ be reduced to the differential equation of the Weierstrass $\mathscr{P}$ function (Abramowitz and Stegun 1965) with $g_3 = 0$ and ξ_0 and g_2 arbitrary constants. In this way, taking into account also the homogeneity relation satisfied by the $\mathscr{P}$ function, the constant K may be eliminated and the (in the OS-sense) separable TW solutions of equation (2) have the form

$$n(Z) = 1 \pm (1-\gamma)^{1/2} w\mathscr{P}^{1/2}(w + w_0, g_2, 0), \tag{10}$$

where $Z = z - ut$, $u = \mp 3[\tfrac{1}{2}(1-\gamma)]^{1/2}$, w_0 and g_2 are arbitrary constants restricted only by the requirement $n(Z) \geq 0$, and

$$w = \exp(-uZ/3). \tag{11}$$

(The $\pm$ signs in u and in front of $(1-\gamma)^{1/2}$ are uncorrelated.)

In the following we should like to pick out from (10) those solutions only, which describe (both spatially and temporally) bounded concentration distributions. The explicit expressions of the $\mathscr{P}$ function for $g_2 \gtrless 0$ and $g_2 = 0$ show (Abramowitz and Stegun 1965) that such concentration distributions only exist for $g_2 = 0$. Indeed, in this case $\mathscr{P}(w + w_0, 0, 0) = (w + w_0)^{-2}$ and thus

$$n(Z) = 1 \pm (1-\gamma)^{1/2} w(w + w_0)^{-1}, \tag{12}$$

where $w_0 \geq 0$ and w is given by equation (11).

Let us now discuss the physical meaning of these solutions. First we notice that, due to the four possible sign combinations, equation (12) yields in general four different solutions which break all the symmetries ($z \to -z$, $z \to z + z_0$, $t \to t + t_0$) of equation (2). For $w_0 = 0$, however, this set reduces to the two stable uniform solutions $n_{1,2}$ given by equation (4), which possess all these symmetries. Further, for finite Z and infinitesimal w_0, equation (12) yields certain (symmetry breaking) solutions of the linearised version of equation (2) around the uniform solutions $n_{1,2}$. For $w_0 > 0$ the solutions (12) only exist in a dynamical regime, i.e. for non-vanishing velocity u (measured in units of $\langle u \rangle = \langle z \rangle / \langle t \rangle$). In this case they describe kink-shaped spatio-temporal concentration distributions. These kinks always carry the concentration field $n(z, t)$ from the unstable uniform state $n_3 = 1$ at $t = -\infty$ into one of the stable uniform states $n_{1,2}$ at $t = +\infty$. Therefore the solutions (12) describe a possible dynamics of the transition from an unstable steady state into a stable one in an open system far from equilibrium.

Finally, we should.like to show that our moving kinks given by equation (12) are related in a subtle manner to the static kinks given by equation (5). With this aim, let us linearise the evolution equation (2) around the static solutions (5) according to

$$n(z, t) = n_s(z) + v(z) \exp(-\lambda t) \tag{13}$$

where $v(z)$ is an infinitesimal quantity and λ a parameter. The linearised equation looks like

$$\frac{d^2 v}{d\zeta^2} + 2 \left(\frac{\lambda}{1 - \gamma} - 2 + 3 \operatorname{sech}^2 \zeta \right) v = 0, \tag{14}$$

where $\zeta = [\frac{1}{2}(1 - \gamma)]^{1/2} z$. This (Schrödinger-like) equation admits only two bounded solutions for $v(z)$. One is the Goldstone mode $v(z) \sim \operatorname{sech}^2 \zeta$ corresponding to $\lambda = 0$, which reflects the marginal stability of the static kinks against translations, and the second is $v(z) = v_0 \sinh \zeta \operatorname{sech}^2 \zeta$ and corresponds to the (positive) eigenvalue $\lambda = 3(1 - \gamma)/2$. Therefore, the static kinks (5) are stable against small perturbations, their single stable mode being of the form

$$n(z, t) = n_s(z) + v_0 \sinh \zeta \operatorname{sech}^2 \zeta \exp \left[-\tfrac{3}{2}(1 - \gamma)t \right], \tag{15}$$

where v_0 is an infinitesimal constant. Hence, for $\zeta \to \pm\infty$, the perturbed static kink (15) behaves as

$$n(z, t) \underset{\zeta \to \pm\infty}{\sim} n_{1,2} \pm 2v_0 \exp \left[\mp\zeta - \tfrac{3}{2}(1 - \gamma)t \right], \tag{16}$$

and its antikink as

$$n(z, t) \underset{\zeta \to \pm\infty}{\sim} n_{2,1} \pm 2v_0 \exp[\mp\zeta - \tfrac{3}{2}(1 - \gamma)t]. \tag{17}$$

Now, it is easy to see that by choosing $|v_0/w_0| = |u|/3\sqrt{2}$, one of the four moving kinks (12) always approaches for $\zeta \to +\infty$ or $-\infty$ one of the stable uniform states $n_{1,2}$ just like the stable mode (15) of the static kink or antikink (5), i.e. according to one of the asymptotic equations (16), (17).

The concentration distributions described by equation (12) are explicit examples for creation of spatio-temporal order in open systems far from equilibrium. Initially the Schlögl model was created to describe the autocatalytic chemical reactions (1) as an example of a system showing a non-equilibrium phase transition. Since then various aspects of this model have attracted considerable interest (for recent contributions

see e.g. Dewel *et al* 1981, Brachet and Tirapegui 1981, Grassberger 1981, Dung and Kozak 1981). In this respect it is interesting to note that the evolution equation (2) of the discussed model is also adequate for the description of the morphogenetic field of a multicellular ensemble (Livshits *et al* 1981) and other synergetic systems.

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