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PATTERN FORMATION IN REACTION DIFFUSION SYSTEMS WITH FINITE GEOMETRY *

Carlos Borzi **
International Centre for Theoretical Physics, Trieste, Italy.

and

Horacio Wio
Centro Atomico Bariloche, 8400–Argentina.

ABSTRACT

We analyze the one–component, one–dimensional, reaction–diffusion equation through a simple inverse method. We confine the system and fix the boundary conditions as to induce pattern formation. We analyze the stability of those patterns. Our goal is to get information about the reaction term out of the preknowledgment of the pattern.

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** Permanent address: IFLYSIB, c.c.565, La Plata (1900), Argentina.

The one–component, one–dimensional, reaction–diffusion equation was recently revisited and profile reaction–rate pairs were generated through a simple inverse method [1]. In that work, travelling wave solutions were found to be stable in unbounded systems, provided the front waves propagated with bounded velocities. We shall use in this letter that inverse method of solution. After confining the system to finite geometries, we shall propose several steady state profiles motivated on different physical problems. We shall find their associated source terms and analyze their stability in front of perturbations. By means of this analysis we shall provide information about the dynamical nonlinear excitation of the media for those cases in which the pattern is (say experimentally) given.

The equation we care about is:

$$u_t(x,t) = Du_{xx}(x,t) + f(u) \tag{1a}$$

where u is the concentration of the species of interest, D is its diffusion coefficient and $f(u)$ some unknown function which quantifies a local source for the diffusing species. As we are considering the steady state situation, we set:

$$u(x,t) = u(x) \tag{1b}$$

which corresponds to a stationary profile.

The inversion procedure, whose details can be found in Ref.[1], works as follows: we first lower the degree of the equation by introducing a new variable

$$\psi(u) = u_x(x) \tag{2a}$$

(that can be done since Eq.(1) is autonomous [2]) and assume that the nonlinearity is only a function of the new variable:

$$f(u) = R(\psi) \tag{2b}$$

(this assumption is not essential but preserves analyticity). Then we invert the role of the variables by setting:

$$u = \phi(\psi)$$

and so,

$$u' = \frac{d\phi}{d\psi} = \frac{-D\psi}{R(\psi)} \,. \tag{3}$$

Note that if we set

$$u^* = \frac{u}{c_\mu}, \quad \psi^* = \frac{\psi L}{c_\mu}, \quad D^* = \frac{Dc_\mu}{L}$$

where c_μ is some reference concentration value and L is a characteristic length of the system, say its one–dimensional size, Eq.(3) is dimensionless.

Case a:

Let us first consider a simplified form for the flux of thermal neutrons [3] in the core of a reactor. We restrict the geometry to $0 < x < 1$ and propose the pattern:

$$\phi(x) = A[1 + \cos(Bx)] \tag{4a}$$

with boundary conditions:

$$\phi'(0) = 0 \quad (\text{or} \quad \phi(0) = 2A), \quad \phi(1) = A[1 + \cos B] \tag{4b}$$

which fix

$$A = \frac{\phi(0)}{2}, \quad B = \cos^{-1}\left(\phi(1) - \frac{\phi(0)}{2}\right) .$$

Following the steps sketched above, we get:

$$\psi(\phi) = \mp AB \left[1 - \left(\frac{\phi}{A} - 1\right)^2\right]^{1/2} \tag{5}$$

and through Eq.(3) with the defintions (2):

$$f(u) = DB^2(u - A) . \tag{6}$$

Let us now analyze the stability of the proposed pattern generated by the reaction rate (6). We set, as usual,

$$\phi(x,t) = \phi_a(x) + \varepsilon(x,t) \tag{7}$$

with ϕ_a coming from (4) and ε some small perturbation. We get

$$\varepsilon_t(x,t) = D\varepsilon_{xx}(x,t) + F_a(x)\varepsilon(x,t) \tag{8}$$

where

$$F_a(x) = \frac{DB}{A} = \text{const} . \tag{9}$$

As Eq.(8) is linear it is separable into product solutions of the form

$$\varepsilon(x,t) = \eta(x)\; e^{-\lambda t} \tag{10}$$

rendering

$$-\lambda\eta(x) = D\eta''(x) + F_a(x)\eta(x) \tag{11}$$

with

$$\eta(0) = \eta(1) = 0$$

and so, $\eta \sim \sin(\mu\pi x)$ and

$$-D\pi^2\mu^2 + \frac{DB}{A} + \lambda_\mu = 0 . \tag{12}$$

The first eigenvalue is the only one which matters

$$\lambda_1 = D\left(\pi^2 - \frac{B}{A}\right) .$$

The pattern will be stable for $\lambda > 0$, that is for $\frac{B}{A} < \pi^2$. $\frac{B}{A} = \pi^2$ locates a critical line in the parameter space.

Case b:

We shall revisit now the Schlögl model for a nonlinear chemical reaction showing a nonequilibrium phase transition [4]. We propose the typical hyperbolic–tangent profile

$$\phi(x) = A\,[\,1 + \tanh\,(Bx)] \qquad (13a)$$

with the boundary conditions

$$\phi(\pm 1) = A[\,1 \pm \tanh\,B] \qquad (13b)$$

for a system confined to $-1 < x < 1$. We obtain

$$\psi = 1 - \left(\frac{\phi}{A} - 1\right)^2 \qquad (14)$$

rendering

$$f(u) = 2\left(\frac{B}{A}\right)^2 D\left\{-u^3 + 3Au^2 - 2Au\right\} \qquad (15)$$

which is the expected cubic nonlinearity.

Let us now analyze the stability of the hyperbolic–tangent pattern. After applying a small local perturbation we re–obtain Eq.(11), the coefficient of $\eta(x)$ in the r.h.s. being now

$$F_b(x) = 2\left(\frac{B}{A}\right)^2 D\left\{-3\phi^2(x) + 6A\phi(x) - 2A^2\right\} . \qquad (16)$$

Again sign (λ) will discriminate the stability of (13). The parameter space will be divided in regions of different regimes characterized for the stability, or not, of the proposed pattern. The critical values of the parameters should be found numerically and they will be reported elsewhere. We shall give here a qualitative argument inspired in the former simple case, which is routine in the theory of thermal neutrons [3]. With that end we homogenize the function $F_b(x)$ by replacing it by its average in the region $-1 < x < 1$, where the system is defined

$$\langle F_b \rangle = \frac{1}{2}\int_{-1}^{1} F_b(x)\,dx = 2\,B^2 D\left[\frac{6\tanh B}{B} - 2\right] . \qquad (17)$$

Stability can be ensured whenever $\langle F_b \rangle < 0$, that is $\lambda > 0$ so if B is small, $\tanh(B) \sim B$ and the pattern is unstable. If B is large enough, $\tanh(B) \sim 1$ and the pattern is stable.

Case c:

We consider now a pattern whose shape is similar to the former one. It has an associated nonlinearity which again corresponds, although now asymptotically, to a Schlögl type of model

$$\phi(x) = A\left[1 + \frac{1}{B}\, tg^{-1}(Bx)\right] \tag{18a}$$

with

$$\phi(\pm 1) = A\left[1 \pm \frac{1}{B}\, tg^{-1} B\right] \tag{18b}$$

so

$$\psi = \frac{A}{tg^2\left[B\left(\frac{\phi}{A} - 1\right)\right] + 1} \tag{19}$$

rendering

$$\begin{aligned} f(u) &= \frac{2\ DAtg\left[\frac{B}{A}(u - A)\right]}{B\left\{1 + tg^2\left[\frac{B}{A}(u - A)\right]\right\}^2} \\ &= a_0 + a_1 u + a_2 u^2 + a_3 u^3 + \ldots \end{aligned} \tag{20}$$

where

$$a_0 = 2\,DAB^2(B^2 - 1); \qquad a_1 = -10\,DB^2\left(B^2 + \tfrac{1}{5}\right)$$
$$a_2 = \frac{10\,B^4}{A}; \qquad a_3 = \frac{10\,DB^4}{3\,A^2}$$

We shall analyze the stability of this profile in the same manner we did with the former one. The coefficient of $\eta(x)$ in the r.h.s. of the analogous of Eq.(11) is now:

$$F_c(x) = \frac{2\,DB^2[\,1 - 4\,B^2x^2 - 4\,B^4x^4\,]}{1 + B^2x^2} \tag{21}$$

The average on $-1 < x < 1$ produces:

$$\langle F_c \rangle = \frac{2}{B}\, tg^{-1} B - \frac{8}{3}\, B^2 \tag{22}$$

so for small B,

$$\langle F_c \rangle \sim \frac{2}{B}\left(B - \frac{B^3}{3} + \ldots\right) - \frac{8}{3}\, B^2 = 2 - \frac{2\,B^2}{3} \sim 2$$

and for large B

$$\langle F_c \rangle \sim \frac{2}{B}\left(\frac{\pi}{2} - \frac{1}{B} + \ldots\right) - \frac{8}{3}\, B^2 \sim -\frac{8}{3}\, B^2\ .$$

As before, the pattern is stable when B is large enough.

Case d:

The last case we shall consider in this letter gives rise to a model for autocatalytic reactions [5]. We propose

$$\phi(x) = A\,\mathrm{sech}^2(Bx) \tag{23a}$$

with boundary conditions

$$\phi(\pm 1) = A\,\mathrm{sech}^2 B \quad \text{or} \quad \phi'(\pm 1) = B \tanh\left[B\phi(\pm 1)\right] \tag{23b}$$

and get

$$\psi = 2B\phi\left(1 - \frac{\phi}{A}\right)^{1/2} \tag{24}$$

which renders:

$$f(u) = \frac{6DB^2u^2}{A} - 4DB^2u \tag{25}$$

The usual stability analysis produces

$$F_d(x) = 4DB^2[3\,\mathrm{sech}^2(Bx) - 1] \tag{26}$$

as the coefficient of the last term in the r.h.s. of the analogous of Eq.(11). Taking the average of F_d on $-1 < x < 1$ we get:

$$\langle F_d \rangle = 4DB(\tanh\, B - B) \tag{27}$$

which is negative, and so the pattern is stable, when B is large enough.

We have considered four cases of one–component one–dimensional reaction–diffusion systems in finite geometries. In those systems, for restricted values of the parameters, spontaneous pattern formation takes place. The simplest one, for which we located a critical line in the parameter space, corresponds to a simplified model for the flux of thermal neutrons in the core of a reactor. The other three cases, which respectively mimic two versions of the Schlögl model for non–equilibrium phase transitions and a simple autocatalityc reaction, were treated in a qualitative fashion. The asymptotic values of the parameters for which the proposed pattern is stable were determined. The critical values of those parameters will be numerically investigated and reported elsewhere.

We stress the fact that in a simple reaction diffusion system in one–dimension, a stable pattern can be generated by the introduction of the proper boundary conditions. The pattern merges out of the balance of the maintained boundary conditions, the diffusion and the contribution of the dynamically distributed sources in the medium. We have provided a procedure for investigating those distributed sources whenever the pattern was known.

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