Stationary states in a reaction–diffusion system with albedo boundary conditions

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Abstract. We study the existence and stability of stationary states in an exactly solvable reaction–diffusion model, under conditions of partial absorption and reflexion at a boundary. The rich variety of time-independent solutions—which, if stable, are candidates to describe the long-time asymptotic state of the system—suggests that such mixed boundary conditions can strongly affect the solution set of more general reaction–diffusion models. This conclusion is relevant in many applications, in particular, in nucleating systems.

In recent years, much attention has been devoted to the study of reaction–diffusion models. This interest is motivated by the relevance of such models in the applications to several areas of science and—from a more fundamental viewpoint—because of their paradigmatic role as self-organizing non-equilibrium complex systems. Indeed, the analytical description of pattern formation in physico-chemical and biological systems is mainly restricted to reaction–diffusion equations [1].

A point of practical interest in the study of the appearance of organized structures in complex systems regards the effect of boundary conditions on their evolution [2, 3]. In this paper, we are concerned with the influence of partial-reflexion (*albedo*) boundary conditions on the existence and stability of stationary patterns in reaction–diffusion systems. To deal with this problem we study an analytically tractable model—the Ballast resistor.

The Ballast resitor reaction–diffusion model [4] describes an electrical device consisting on a superconducting wire with critical temperature T_c, carrying a constant current I and immersed in a heat bath at constant temperature T_0. According to the energy balance at each point along the wire, the local temperature can be below or above the critical value T_c. Therefore, at a given time, the temperature profile on the wire consists of structured zones of normal or superconductor phase. Energy conservation implies that the temperature field $T(x, t)$ satisfies the reaction–diffusion equation

$$\partial_t T - \partial_x^2 T = -T + T_h \Theta(T - T_c) \tag{1}$$

where $\Theta(T - T_c)$ is a Heaviside step function describing the temperature dependence of resistivity, and $T_h \propto I^2$ acts as an external control parameter. We have used dimensionless spatial and temporal variables, assuming that the specific heat of the wire, its heat conductivity and the heat transfer rate to the bath are constants. Moreover, without loss of generality, we have taken $T_0 = 0$.

The reaction terms in (1) are piecewise linear. This fact makes it possible to treat the problem analytically, although preserving its nonlinear character [5]. Besides describing the

Ballast resistor, the equation can be seen to represent a mimic of the well known Schlögel model of bistable reaction kinetics [6]. In this case, the field $T(x, t)$ would represent the density of the relevant chemical species.

We are interested in the stationary solutions of (1), which satisfy

$$\frac{d^2 T}{dx^2} = T - T_h \Theta(T - T_c).$$ (2)

We concentrate in the case $T_h > T_c$, as this condition permits the existence of non-trivial solutions. For an infinite system $(-\infty < x < +\infty)$, the only bounded solutions to this equation are constant, $T(x) = 0$ and $T(x) = T_c$. In fact, according to

$$z = 1 - 2T_c/T_h$$ (3)

being positive or negative, the solution to the time-dependent problem—which has the form of a travelling wave—asymptotically approaches one of those states. The same problem in a finite domain has been treated in detail in [5].

Here, we consider instead a semi-infinite system in the positive x-axis. For this second-order differential problem, the most general (linear) boundary condition at $x = 0$ is a homogeneous combination of the distribution T and its derivative,

$$\left[\frac{dT}{dx} - kT \right]_{x=0} = 0.$$ (4)

In the Ballast model, this albedo boundary condition represents a partial absorption and reflexion of energy flux at the origin. The extreme cases, $k \to 0$ and $k \to \infty$, correspond respectively to vanishing heat flux $(dT/dx|_{x=0} = 0$, Neumann boundary condition) and to vanishing temperature $(T|_{x=0} = 0$, Dirichlet boundary condition). These cases are analysed in [3]. Intermediate values of the albedo parameter describe a partially isothermic and adiabatic contact at the wire end. This interpretation can be straightforwardly extended to the case of chemical reactions, where $T(x)$ represents a stationary particle density.
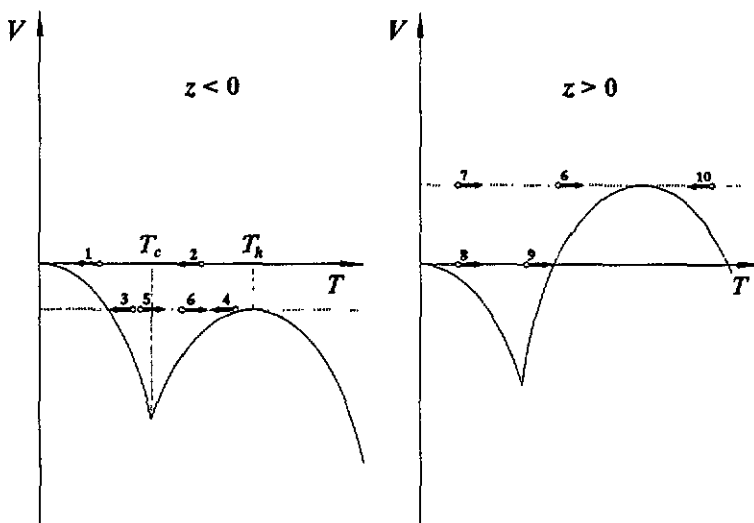

Figure 1. Mechanical potential and initial conditions for various solutions with albedo boundary, in the mechanical analogy of (2).

In order to analyse the existence of stationary states we exploit a mechanical analogy of (2). Associating T with position and x with time, this equation represents Newton's law for a particle of unitary mass under the action of the potential

$$V(T) = \begin{cases} -T^2/2 & \text{if} \quad T < T_c \\ -T^2/2 + T_h(T - T_c) & \text{if} \quad T > T_c. \end{cases} \tag{5}$$

In this analogy, the albedo boundary condition implies that at the initial time, $x = 0$, the particle velocity is given by its position times the albedo parameter k. This condition implies that not all the trajectories of the particle are acceptable as solutions of our problem.

In figure 1 we plotted, along with the shape of the potential $V(T)$, the initial values of T, the total energy, and the initial velocity direction for each type of solutions we were able to find under albedo boundary conditions. These types differ not only in the shape and in the value of the solution $T(x)$, but also in the range of the parameters k and z where they exist. Figure 2 shows the domains of existence for each type in the (k, z) plane, and in figures 3(a) and 3(b) we plot a schematic graph of these solutions. Numbering is in correspondence with figure 1.
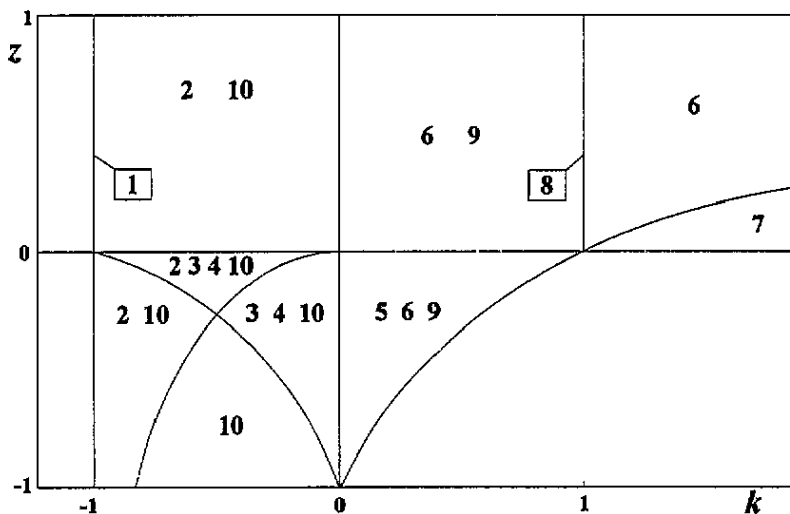

Figure 2. Existence domains of the solutions shown in figure 1, in the (k, z) space. Solutions number 1 and 8 exist on the lines $k = -1$ and $k = 1$, respectively.
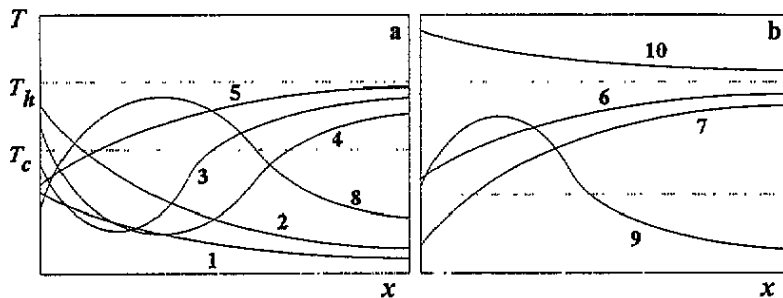

Figure 3. Schematic representation of the stationary solutions shown in figure 1, as functions of the space coordinate x; (a) unstable states, (b) stable states.

In these figures, we have not taken into account the trivial stationary solution $T(x) = 0$, which exists for any value of k and z.

Observe that, from physical considerations, we have required that the solution $T(x)$ be bounded for all x. We have also discarded the unrealistic oscillatory solutions which, in the mechanical analogy, correspond to intermediate energies, between the minimum and the lowest maximum of $V(T)$.

Except for the trivial solution, no bounded stationary state exists for $k < -1$. This can be interpreted in physical terms from the fact that a negative albedo parameter represents a boundary in which the reflected heat flux is greater than the incident one. In this case, energy is being continuously injected into the system from outside through the contact. Therefore, if the injection rate is too large (k too negative), dissipative effects fail to keep the wire temperature bounded.

The explicit forms of the stationary temperature distributions $T(x)$ can be found by direct integration of (2) and, for the sake of conciseness, are not included here. The piecewise-linear character of the equation implies that the solution is pieced together from exponential portions. These portions have to be matched by equating their values and derivatives at the critical coordinate x_c, defined by $T(x_c) = T_c$. Therefore, the problem is essentially a linear algebraic one, although it can become rather complex for solutions such as numbers 4 and 8, which have two critical coordinates.

Form (1), linear stability analysis of the time-independent solutions leads to the following equation for the perturbation from the stationary state, $\psi(x, t)$:

$$\partial_t \psi - \partial_x^2 \psi = [-1 + T_h \delta(T - T_c)] \psi . \tag{6}$$

In this linear reaction–diffusion equation, the delta function on T can be replaced by $\delta(x - x_c)$, once the critical coordinate x_c is known. For the solutions with two critical coordinates, $\delta(T - T_c)$ has to be replaced by a sum of two delta functions on x.

Proposing $\psi(x, t) = \exp(\lambda t) \Psi(x)$, the solution for $\Psi(x)$ is piecewise exponential. The pieces are matched requiring continuity of Ψ and a finite discontinuity in its derivative, due to the delta function in x_c. The sign of λ determines the stability of the stationary solution.

From this analysis it turns out that the states shown in figure 3(a) are unstable, whereas those plotted in figure 3(b) are stable. The trivial stationary solution is stable for $k > 0$ and unstable otherwise. This can be easily understood observing that for $k < 0$, as soon as the temperature field is positive at the boundary, there is a net heat flux entering the system. For $k > 0$ instead, heat is absorbed at the contact and the temperature tends to decrease.

As a rule, under conditions of coexistence of stationary solutions, stability is observed in the states which present the smaller zones of superconductor phase. The dissipation in the normal phase seems to stabilize the structure of the temperature field. However, for $k > 0$, there are several zones of multistability (compare figures 2 and 3(b)), in which some of the states 6 to 9, as well as the trivial solution $T(x) = 0$, are simultaneously stable. Hence, in the whole evolutionary problem governed by (1), the asymptotic temperature profile will be selected by the initial condition. On the other hand, for negative albedo, the only stable solution is number 10. This high-temperature distribution is the only state able to dissipate the heat flux entering the wire through its end.

Among the stable states depicted in figure 3(b), numbers 7 and 9 deserve particular consideration. These structures present a change of phase between a finite region adjacent to the boundary and the remaining of the wire. Near $x = 0$, state number 7 is in the superconducting phase and state number 9 is in the normal phase. At the critical point x_c they cross the critical value T_c and invert their phase. The temperature profiles of these

states are, respectively, given by

$$
T_7(x) = \begin{cases}
\dfrac{1}{2\eta} T_h \left[\exp(x) + \dfrac{1-k}{1+k} \exp(-x) \right] & \text{for } x < x_c \\[3mm]
T_h - \dfrac{1}{2} T_h \left[\eta + \dfrac{1-k}{\eta(1+k)} \right] \exp(-x) & \text{for } x_c < x
\end{cases}
\tag{7}
$$

and

$$
T_9(x) = \begin{cases}
T_h - \dfrac{1}{2\eta} T_h \left[\exp(x) + \dfrac{k-1-2k\eta}{1+k} \exp(-x) \right] & \text{for } x < x_c \\[3mm]
\dfrac{1}{2} T_h \left[\eta + \dfrac{k-1-2k\eta}{\eta(1+k)} \right] \exp(-x) & \text{for } x_c < x
\end{cases}
\tag{8}
$$

where $\eta = \exp(x_c)$. For state number 7, $\eta = \left[(k-1)/z(k+1) \right]^{1/2}$, and for state number 9 we have $\eta = \left[2k + \left(4k^2 - 4z(k^2-1) \right)^{1/2} \right]/2z(1+k)$.

In a generalized interpretation of the Ballast model, these two-phase distributions can be seen as the result of two competing processes, namely, *nucleation*—which tends to enlarge the finite region near the boundary by aggregation—and *evaporation*—which induces this nucleation zone to shrink. But it is well known that nucleating systems not subject to boundary conditions are completely unstable [7]. In free space, a nucleating region either grows catastrophically due to the prevailing of aggregation, or shrinks up to disappearance by evaporating. With albedo boundary conditions, instead, we see that a non-trivial stable stationary state does exist. If this structure succeeds to be that asymptotic distribution in the time-dependent problem, equation (1), we can assert that such boundary conditions are able to stabilize the nucleation process, even in a semi-infinite domain.

The rich variety of stationary states found for the simple reaction–diffusion model considered here under albedo boundary conditions—in particular, compared with the free-space case, and even with the limits of Dirichlet and Neumann boundaries—suggests that, generally, albedo introduces non-trivial features in the evolution of similar systems. Except for a few previous works [5, 2], this point seems to have passed unnoticed in the study of reaction–diffusion processes. However, in view of the relevance of boundary conditions in actual applications of those processes [1]—and, in particular, regarding recent experimental results on reflexion and refraction of chemical waves [8]—it is indeed worth considering these more realistic boundary conditions.

Acknowledgments

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