Nucleation structures in reaction-diffusion-convection systems

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The existence and stability of one-dimensional structures in reaction-diffusion systems subject to convection velocity fields are studied analytically and numerically. Attention is focused on nucleation patterns—which exhibit a well defined, localized accumulation of particles—in bistable reaction models. It is shown that a sufficiently strong, implosive convection field is able to stabilize those patterns, which are generally unstable in reaction-diffusion systems. Such velocity fields and the stabilization mechanisms are characterized and some exact solutions of stable and unstable structures in these reaction-diffusion-convection models are presented.

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I. INTRODUCTION

Reaction-diffusion (RD) models have been extensively used to describe physical systems [1] such as chemical reactions [2], combustion [3], and electrothermal processes [4]. They have also been applied in other branches of science, particularly, in biology, where they are used as models for morphogenesis and population dynamics [5]. Their interest is not only related to specific applications, but is also due to the fact that RD processes are paradigmatic of complex behavior, as they can exhibit, for instance, self-organization, spatiotemporal pattern formation, and chaotic evolution [6].

For one-component systems, RD models are described by the nonlinear partial differential equation

$$\partial_t n = D\nabla_{\mathbf{r}}^2 n + \gamma F(n), \tag{1}$$

where $n(\mathbf{r},t)$ is the relevant field, typically, a particle density. The source of nonlinearity in this equation is the function $F(n)$, which stands for the density-dependent source due to reaction processes. The positive coefficient γ measures their relative strength with respect to diffusion, characterized by the diffusivity D.

A class of reaction models that has attracted considerable interest because of its application to the analysis of pattern formation are the bistable reactions [1]. In these reactions, the spatially homogeneous rate equation $\dot{n} = F(n)$ has two stable stationary states, corresponding to two solutions of $F(n) = 0$ at which $F'(n)$ is negative. Usually, between these two stable states there is an unstable one, with $F'(n) > 0$, situated at the limit of the basins of attraction of the stable solutions. A characteristic example of these bistable reactions is the Schlögl model [7]

$$F(n) = (n_1 - n)(n_2 - n)(n_3 - n) \tag{2}$$

($n_1 < n_2 < n_3$), where the stable states are n_1 and n_3.

In the spatially dependent problem described by Eq. (1), bistable reactions determine the system to behave in a typical way, practically independent of the initial condition and the values of D and γ [8]. In fact, during the first stage of the evolution, spatial domains develop, at which $n(\mathbf{r},t)$ adopts a practically constant value coinciding with one of the stable solutions of the homogeneous rate equation. In the second stage, the evolution consists mainly in the shock-front-like motion of domain interphases [9], with steady growth or shrinkage of the domains. Eventually, one of the two phases dominates and the density $n(\mathbf{r},t)$ becomes finally homogeneous. As a consequence of this typical behavior, it is concluded that *no stable spatial structures can develop in a bistable reaction-diffusion system*, at least in free space [4].

A particular case of this conclusion is a well known property of nucleating systems [10], which applies, for instance, to phase transitions of the gas-liquid type. Under fairly general conditions, nucleation is an unstable process: once a nucleating center has formed, the condensed (liquid) phase region either grows indefinitely—dominating over the diluted (vapor) phase—or shrinks and disappears.

Is it possible to stabilize nucleation or other spatial patterns in bistable reacting and diffusing systems by a proper modification of the underlying transport process? The answer to this question—the goal at which we aim in this paper—has to do with the more general problem of interplay of reaction and transport mechanisms other than diffusion. In particular, we are interested in considering convective transport, which should play a relevant role in the behavior of reacting fluids, combustion, atmospheric dynamics, and other physical systems [11–13]. The present paper is therefore devoted to study the existence and stability of nucleation-type structures in reacting, diffusing, and convecting (RDC) systems. It is organized as follows. In the next section the model equation is presented and patterns associated with nucleation are characterized. In Sec. III, we show that the spatial asymptotic behavior of the stationary solutions to the model equation determines their existence. Next, the stability of the stationary patterns, related to the

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development of shock structures in the RDC system, is studied both analytically and numerically. Some exact solutions, in the frame of the so-called Ballast reaction model [4], are presented in Sec. V. Finally, we summarize our results in Sec. VI.

II. THE REACTION-DIFFUSION-CONVECTION MODEL: NUCLEATION PATTERNS

As a first approach to the study of nucleation structures in RD systems subject to convection, we consider a one-dimensional system of reacting and diffusing particles, passively transported by a velocity field $v(x)$. This implies that the convective flow is not affected by reactions and therefore $v(x)$ can be considered as a given field. A more general treatment would imply the consideration of an evolution equation for the velocity field and, eventually, for higher-order velocity moments, such as temperature or pressure [13].

Within the hypothesis of passive transport, the one-dimensional version of Eq. (1) generalized to consider convection reads [12]

$$\partial_t n + \partial_x (vn) = D\partial_x^2 n + \gamma F(n). \tag{3}$$

As in the case of Eq. (1), the formulation of this RDC equation is essentially phenomenological. Stationary solutions to Eq. (3) satisfy the ordinary differential equation

$$(vn)' = Dn'' + \gamma F(n), \tag{4}$$

where the primes indicate differentiation with respect to x.

According to the discussion in the Introduction, we shall consider a bistable reaction model, qualitatively similar to Eq. (2). For simplicity, and without loss of generality, we suppose that the lower stable state of the reaction process is $n_1 = 0$. Nucleation structures will therefore be associated with a density domain where $n(x,t)$ is near the higher stable value n_3. We shall call such a domain the *condensed* region. Outside the domain, in the *diluted* region, the density should decrease to zero.

We expect that, in order to avoid the indefinite growth or shrinkage observed for density domains in RD systems, the convection velocity field able to stabilize such patterns should be implosive or explosive, respectively. In an implosive (explosive) field, in fact, velocity is directed "inward" ("outward") and it may be able to resist the ustable combined effect of reaction and diffusion over a density domain near the implosion (explosion) center. In view of this, and with the aim of simplifying the mathematical problem, we consider implosive and explosive symmetric velocity fields centered at $x = 0$:

$$\begin{aligned} &v(x) = -v(-x) < 0 \quad \text{for } x > 0 \text{ (implosive)} \\ &v(x) = -v(-x) < 0 \quad \text{for } x < 0 \text{ (explosive)}. \end{aligned} \tag{5}$$

Although studying implosive and explosive velocity fields only could seem a severe restriction on the applicability of our results, it is worthwhile to observe that, at least locally, practically every velocity field has a well defined implosive or explosive character. Indeed, an arbitrary $v(x)$ can be expanded around a given (regular) point x_0 as $v(x) \approx v(x_0) + \omega_0(x - x_0)$, with $\omega_0 = dv/dx|_{x_0}$. Therefore, except for the constant term $v(x_0)$, which acts as a locally homogeneous drift, $v(x)$ is implosive (explosive) if ω_0 is negative (positive). In view of this, we expect our results to be useful in the description of a wide class of situations, at least in an approximate way.

We shall consider here symmetric density fields $n(x,t) = n(-x,t)$, which will produce symmetric stationary nucleation patterns. These symmetry properties in $v(x)$ and $n(x,t)$ make it possible to restrict the problem to the positive x axis, with the boundary condition

$$v(0)n(0,t) = D\partial_x n(0,t), \tag{6}$$

which can be obtained by integrating Eq. (3) around $x = 0$. Note that, at the origin, $n(x,t)$ is a continuous function, whose derivative can present a finite discontinuity if the velocity field is also discontinuous.

A relevant condition to impose over the nucleation structures in order to represent a well defined, physically meaningful accumulation of particles is to involve a finite particle number, i.e.,

$$\int_{-\infty}^{+\infty} n(x,t)\, dx = 2\int_0^{+\infty} n(x,t)\, dx < \infty. \tag{7}$$

This restriction completes the characterization of the density patterns that we shall consider in the following.

III. EXISTENCE OF NUCLEATION PATTERNS: ASYMPTOTIC ANALYSIS

In the analysis of the possibility of stabilizing RD patterns with a convection field, a reasonable first step is to ask about the situation when reactions are completely neglected. In fact, diffusion by itself is unable to produce stationary spatial structures; on the contrary, it tends to eliminate inhomogeneities. Is a velocity field able to compete with this effect, producing stable stationary structures? The answer is "yes." Setting $\gamma = 0$ in Eq. (4), its solution with the boundary condition (6) reads

$$n(x) = n(0)\ \exp\left[\frac{1}{D}\int_0^x v(x')\, dx'\right], \tag{8}$$

where the density at the origin $n(0)$ is an arbitrary positive constant. A straightforward linear stability analysis of this solution shows that it is stable.

The solution (8) can be related to the RDC nucleation patterns only if the density field satisfies $n(x) \to 0$ for $x \to \infty$. As a necessary condition, this implies that $v(x)$ must be negative for $x > 0$. Therefore, as could be expected, the kind of structures we are interested in occur, in the absence of reactions, for implosive velocity fields. Supposing that $v(x)$ does not have nonintegrable singularities, whether the condition of integrability (7) is satisfied depends on the asymptotic large-x behavior of the velocity. We analyze here the asymptotic power-law forms $v(x) \to -Ax^\alpha$ $(A > 0)$, as they are representative of the possible instances of integrability of $n(x)$. Making the power α vary over the whole real domain, these forms of $v(x)$ could give a reasonable idea of the behavior of the system under the effect of more general velocity fields. Three cases can be distinguished.

(i) $\alpha > -1$. In this situation, the large-x spatial dependence of the density is $n(x) \propto \exp\left[-Ax^{\alpha+1}/D(\alpha+1)\right]$ and therefore $n(x)$ is always integrable.

(ii) $\alpha < -1$. In this case, for $x \to \infty$, $n(x)$ has the same form as before but, since $\alpha + 1 < 0$, the density approaches a constant and cannot be integrated in the diluted region.

(iii) $\alpha = -1$. In this marginal case, in which the constant A has units of a diffusivity coefficient, the density behaves as $n(x) \propto x^{-A/D}$ and its integrability depends on the relative value of A and D. It is integrable for $A > D$, i.e., when velocity dominates over diffusion and vice versa.

Having a complete solution for the diffusion-convection system, the original RDC problem can be envisaged from an alternative viewpoint: How do reaction processes affect the existence and stability of diffusion-convection nucleation-type structures? In order to answer the question about existence, we note that, upon very general conditions on $v(x)$ and $F(n)$, the solution to the ordinary differential equation (4) with $\gamma \neq 0$ does exist [14], although finding its analytical form could be impossible in practice. According to Eq. (7), the association of such a solution with a nucleation pattern depends only on its integrability, which is again related to its asymptotic behavior in the diluted region.

For large x, the density is expected to asymptotically vanish, so that the effect of reactions in that limit is determined by the form of $F(n)$ near the stable state $n = 0$. We suppose here that, for $n \to 0$, $\gamma F(n)$ goes as $-\gamma_0 n$ $(\gamma_0 > 0)$, so that the asymptotic analysis can be carried out on the linear equation

$$-A(x^\alpha n)' = Dn'' - \gamma_0 n, \tag{9}$$

where we have taken for $v(x)$ the same asymptotic form as in the diffusion-convection case.

The results of this analysis are summarized as follows.

(i) $0 < \alpha \neq 1$. The contribution of reaction processes to $n(x)$ consists of an exponential factor of the type $\exp(-Bx^{\alpha-1})$ (B is a constant). Hence the large-x behavior of $n(x)$ coincides with the diffusion-convection result

$$n(x) \propto \exp\left(-\frac{A}{D}\frac{x^{\alpha+1}}{\alpha+1}\right). \tag{10}$$

(ii) $\alpha = 1$. In this particular case,

$$n(x) \propto x^{-\gamma_0/A} \exp\left(-Ax^2/2D\right). \tag{11}$$

An exact solution of this type will be presented in Sec. V.

(iii) $-1 < \alpha \leq 0$. For these weaker velocity fields, the reactions enter the asymptotic behavior of the density through an exponential factor that, in fact, dominates over the reaction-convection contribution:

$$n(x) \propto \exp\left(-\sqrt{\frac{\gamma_0}{D}}x\right) \exp\left(-\frac{A}{2D}\frac{x^{\alpha+1}}{\alpha+1}\right). \tag{12}$$

In the limit $\alpha = 0$ the density decays in a purely exponential way $n(x) \propto \exp\left[-\left(A + \sqrt{A^2 + 4\gamma_0 D}\right)x/2D\right]$, as in one of the exact solutions presented in Sec. V.

(iv) $\alpha = -1$. In this marginal situation, the exponential factor found in the previous case appears again:

$$n(x) \propto x^{-A/2D} \exp\left(-\sqrt{\frac{\gamma_0}{D}}x\right). \tag{13}$$

This case will be also considered when analyzing some exact solutions.

(v) $\alpha < -1$. Finally, for these very weak velocity fields, reaction processes completely determine the asymptotic decay of $n(x)$ and the effect of $v(x)$ results to be irrelevant. We find

$$n(x) \propto \exp\left(-\sqrt{\frac{\gamma_0}{D}}x\right). \tag{14}$$

From the mathematical viewpoint, it is interesting to note that these asymptotic decays do not reduce in all cases to the diffusion-convection results as $\gamma_0 \to 0$. This is due to the fact that the appearance of the reaction term changes the order of the stationary RDC equation (4), which, for $\gamma = 0$, is essentially a first-order one.

According to the results of this asymptotic analysis, we see that when reaction processes do act the stationary solutions to the RDC problem are integrable for all values of α and therefore can be acceptably associated with nucleation structures. It is worthwhile to remark that for $\alpha \leq 0$ the integrability is completely determined by the reaction term and does not depend on the sign of the constant A, i.e., on the sign of the velocity field. For positive α, instead, integrable stationary structures occur only for implosive fields, as in the reaction-convection problem.

In summary, stationary solutions of the nucleation type in the RDC problem with bistable reactions are possible, at least for a wide class of velocity fields. The main question, i.e., whether such structures are stable or not, still subsists, however. Its answer is outlined in the next section.

IV. STABILITY OF PATTERNS: SHOCK-FRONT DYNAMICS

Analyzing the stability of the stationary solutions to a nonlinear partial differential equation of the type of (3) usually requires knowing first the explicit form of those solutions. Unfortunately, we cannot expect to obtain the exact stationary densities $n(x)$ from Eq. (4) for general forms of the velocity field and the function $F(n)$. As shown in Sec. V, the stationary equation admits analytical solution only for a few very special forms of $v(x)$ and within a particularly simplified reaction model. Such solutions are often given in terms of complicated special functions. Therefore, most of the conclusions presented in this section, which mainly concern the stability of the stationary solutions, are based on a numerical resolution of Eq. (3). The numerical algorithm consists of a finite difference scheme, which, with a suitable choice of spatial and temporal increments, proves to be fairly stable.

As stated in the Introduction, the dynamics of bistable RD systems for moderately large times is governed by the motion of domain interphases, which, after a short transient, develop a well defined shock-front shape and move at constant speed. This behavior is the main source of the instability that characterizes stationary structures in such systems. It is therefore reasonable to ask, as a first step in considering the stability problem in the full RDC model, what kind of evolution characterizes the motion of interphases between condensed and diluted domains when a velocity field is superposed to the diffusive transport.

In order to answer this question, consider first a constant, space-independent velocity field. In this situation, we propose a similarity solution to Eq. (3), namely a shock front of the form $n(x,t) = n(x - ct) \equiv n(\xi)$. The RDC equation for this solution can be written as

$$(-c + v)n' = Dn'' + \gamma F(n), \qquad (15)$$

where the primes indicate differentiation with respect to ξ. Requiring that $n(\xi) \to n_\pm$ sufficiently far from the front, where either $n_- = n_1$ and $n_- = n_3$ or vice versa, Eq. (3) can be multiplied by n' and integrated over the ξ domain to provide an approximated evaluation of the shock-front speed c [8,13],

$$c = v - \frac{\gamma\Delta}{(n_+ - n_-)^2} \int_{n_-}^{n_+} F(n)\, dn = v + c_0, \qquad (16)$$

where Δ is the width of the front and c_0 is its velocity for $v = 0$. This result indicates that, as we could expect, the constant velocity field is simply superposed to the front speed of the RD system. Some exact solutions to Eq. (15) with $v = 0$ in the frame of simple reaction models [4] show that the front width Δ is essentially equal to $\sqrt{D/\gamma}$ and does not depend on the value of c_0. In fact, the shape of the shock front is determined by the interplay of reaction and diffusion and the front speed c_0, which is proportional to $\sqrt{\gamma D}$, only characterizes the motion of the interphase. As a consequence, we do not expect Δ to be modified by the superposition of the constant velocity v.

Numerical calculations show that, even for a space-dependent field $v(x)$, the front width is practically not modified by the velocity, at least for moderate values of v. This can be understood by taking into account that, although velocity gradients would tend to spread or concentrate the density front, reactions do modify the density by "creating" or "annihilating" particles and, as before, it is their interplay with diffusion that ultimately determines the front shape. Therefore, as a first approximation, the front speed can be put in terms of $v(x)$ as a straightforward superposition of the velocity field and c_0, $c(x) = c_0 + v(x)$. Again, this approximation can be confirmed by numerical means.

The approximated form for the shock-front speed in a velocity field $c = c_0 + v$ makes it clear that $v(x)$ will be able to stabilize the otherwise unbounded motion of the front if there is a point at which $v(x) = -c_0$ and the front is directed toward it. In terms of the stationary structures we are interested in, it can be said that a nucleation center will develop an outgoing shock front depending on the relative values of c_0 and $v(x)$ at the initial condensed region, more precisely, if $c_0 > -v(x)$. Then the unbounded growth of this domain will be stopped only if $v(x)$ is an implosive field, whose modulus grows with x, such that at a certain point $|v(x)| = c_0$. In any other situation, either for an implosive velocity field with decreasing modulus or for an explosive $v(x)$, a growing nucleation center will not be stabilized.

The situation is very different when, in its initial evolution, the condensed region begins shrinking. If the original nucleation center is large enough, an incoming shock front could develop, which would be stabilized by an explosive velocity field at a point where $v(x) = |c_0|$. The identification of such an stable pattern with a nucleation structure would depend on the particular form of $v(x)$ in the diluted region, according to the discussion in Sec. III.

However, in view of the kind of real situations in which nucleation patterns could appear, such as, for instance, vapor-liquid-like phase transitions, we are mainly interested in describing initial conditions with a relatively small condensed region. Under these circumstances, if the initial region begins to shrink, there is no time available to develop a shock front. Numerical simulations show that, even in this case, stable stationary solutions do exist if the velocity field is implosive. Contrary to the previous cases, these stable structures show no features similar to stationary shock fronts and they are typically characterized by a highly populated, small condensed region at the origin. The mechanism that makes the nucleation structures stable in this case is different from the stabilization of shock fronts, as its does not consist simply in opposing advection to the shock motion. Here the large value of $n(x)$ at the nucleation center, always exceeding the high-density stable state n_3, would tend to decrease by the combined action of chemical reactions and diffusion. However, this central region is constantly being fed by the implosive velocity field, which transports particles from the diluted phase. These two opposite trends can compensate each other and produce a stationary stable state consisting of a sort of net density "circulation" between the interior and the exterior of the nucleation center.

Figures 1–3 show some instances of the situations analyzed in this section. In Fig. 1 the relative values of n_2 and n_3 enable the formation of an outgoing shock front from a highly concentrated initial nucleation center. The implosive velocity field is constant and therefore its value is simply superposed to the shock-front speed. As a consequence, after a short transient, the shock front moves at constant speed and the nucleation center grows indefinitely. Note the density spike at $x = 0$, due to the finite

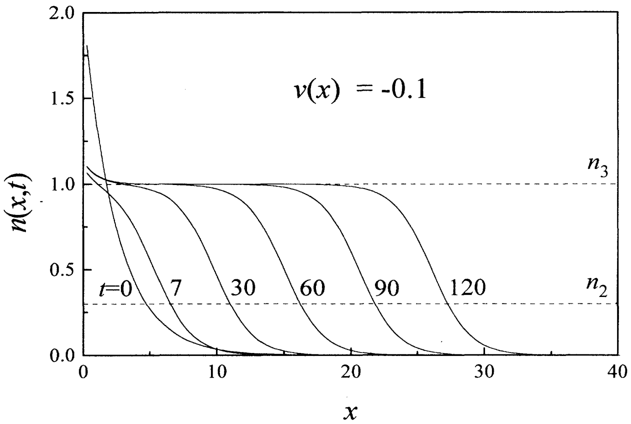

FIG. 1. Numerical solution for the evolution of the density $n(x,t)$ of a reaction-diffusion system in the presence of a constant implosive convection field. The bistable reaction model determines the appearance of an outgoing shock front whose speed is superposed to the convection velocity. Both n and x are given in the units determined by the choice of the parameter values.

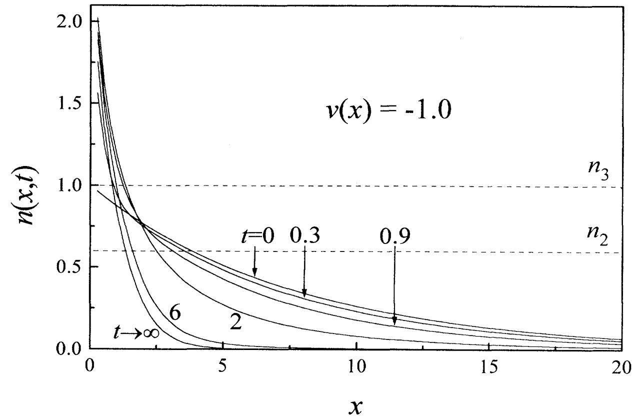

FIG. 3. Here the relative values of n_2 and n_3 determine that the initial condensed region shrinks without forming a shock front. The system reaches a highly concentrated stable state according to the density circulation mechanism described in Sec. IV.

value of $v(x)$ at that point. Regarding diffusion and reaction processes, Fig. 2 shows a similar situation. The difference is now that $v(x)$ grows linearly with x. Hence, at a given point, this implosive velocity field will be able to stop the shock front, stabilizing the growth of the condensed region. Finally, Fig. 3 depicts a case in which the values of n_2 and n_3 produce an initially shrinking nucleation center. The density near the origin grows due to the implosive constant velocity field and the mechanism described in the previous paragraphs begins to act. After a certain time, the stationary state has been practically reached.

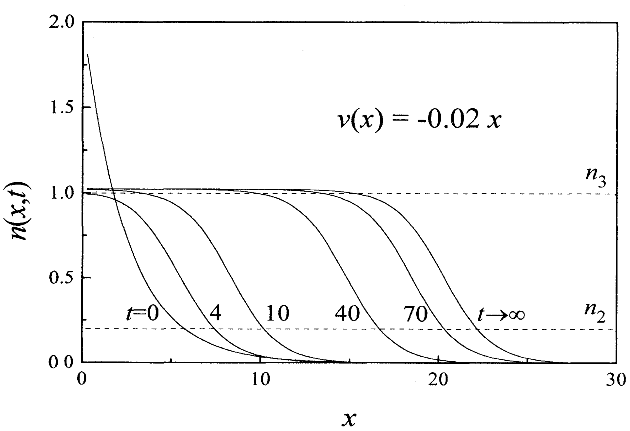

FIG. 2. Same in Fig. 1, but for an implosive velocity field whose modulus grows with x. Now the shock-front speed decreases as the front moves. Asymptotically, the shock front stops and the system reaches a stationary state in the form of a stable nucleation structure.

V. SOME EXACT SOLUTIONS: THE BALLAST MODEL

As pointed out above, an explicit stability analysis of a stationary solution to a given dynamical system usually requires knowing the exact form of such a solution. Exact solutions are also interesting as they facilitate the study of parameter dependence. In one-species reaction-diffusion problems, exact stationary solutions are practically restricted to the Ballast reaction model [4]. In this model, the reaction term is piecewise linear

$$F(n) = -n + n_3 \Theta(n - n_2), \tag{17}$$

where $\Theta(n)$ is the Heaviside step function. This reaction model, which has stable stationary states at $n = 0$ and $n = n_3$, can be seen as a linearized mimic of the Schlögel model Eq. (2). Its piecewise linear form makes it possible to treat analytically the corresponding reaction-diffusion equation in separate spatial domains, which is then matched with appropriate continuity conditions. On the other hand, due to the discontinuity of $F(n)$ at $n = n_2$, the Ballast model essentially preserves a nonlinear character and therefore provides a suitable frame to discuss more general forms of $F(n)$.

In connection with some of the cases analyzed is Secs. III and IV, we present in the following the exact solutions to Eq. (4) for three forms of the convection field $v(x)$. In the first place, we study a linear implosive velocity field $v(x) = -x/\tau$, where $\tau > 0$ is a characteristic time scale. According to the previous discussion, such a velocity field should be able to stabilize outgoing shock fronts. Within the Ballast model Eq. (17), the stationary RDC equation in the diluted region ($n < n_2$) reads

$$0 = \tau D n'' + x n' + (1 - \gamma\tau) n. \tag{18}$$

As for the condensed region, it can be readily seen that

$\eta = \gamma\tau n_3/(\gamma\tau - 1) - n$ also satisfies Eq. (18). Taking $n(x) = \exp(-x^2/4D\tau)u(x)$, the equation for $u(x)$ is solved by the parabolic cylinder or Whittaker functions, which can in turn be put in terms of the confluent hypergeometric functions $U(a,b,c)$ and $M(a,b,c)$ [15].

Taking into account the boundary condition at $x = 0$, Eq. (6), and an appropriate density decay for $x \to \infty$, the density profile for this linear velocity field is

$$n(x) = \begin{cases} a\exp(-x^2/2D\tau)U(\gamma\tau/2, 1/2, x^2/2D\tau) & \text{for } x > x_2 \\ \gamma\tau n_3/(\gamma\tau - 1) - b\exp(-x^2/2D\tau)M(\gamma\tau/2, 1/2, x^2/2D\tau) & \text{for } x < x_2, \end{cases} \tag{19}$$

where x_2 is the (unknown) point at which $n = n_2$. The constants a and b are determined by requiring continuity of $n(x)$ and its derivative at $x = x_2$. These conditions provide linear equations for a and b in terms of x_2. Then, the equation $n(x_2) = n_2$ can be used to obtain the value of x_2. This is a highly complicated equation, which has to be treated numerically. An alternate way to treat this problem consists in calculating the values of n_2 by fixing x_2. This has been done in Fig. 4 to illustrate the type of solutions obtained.

In the diluted region, the solution (19) decays as predicted by Eq. (11) in Sec. III. Furthermore, once the complete form of the stationary solution is known, its stability can be numerically evaluated by means of the usual linearization scheme. As expected from the discussion in Sec. IV, stability results when the reaction parameters n_2 and n_3 determine the existence of outgoing shock fronts.

Curve 1 in Fig. 4 corresponds to the solution (19) with $D = 1$, $\gamma = 1$, $\tau = 5$ $n_3 = 1$, and $x_2 = 8$, which implies $n_2 \approx 0.21$. Although the value of x_2 is not very large as compared with the shock-front width, the appearance of such a structure is apparent. The point at which it has stopped due to the implosive velocity field agrees acceptably with the approximate evaluation presented in Sec. IV.

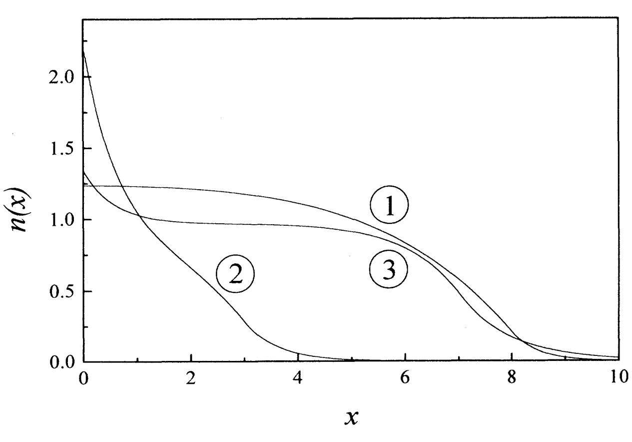

FIG. 4. Some exact stationary solutions for the Ballast reaction model. Curves 1 and 2 correspond to stable nucleation patterns produced by the stabilization of a shock front and the density circulation mechanism, respectively. Curve 3 is a shock-front-shaped unstable structure.

As a second instance in the form of $v(x)$ we consider now a constant implosive velocity field $v(x) = -v$, with $v > 0$. The stationary RDC equation in the diluted region reduces in this case to a second-order ordinary differential equation with constant coefficients

$$0 = Dn'' + vn' - \gamma n. \tag{20}$$

In the condensed region $\eta = n_3 - n$ satisfies the same equation. The solution to the RDC stationary problem is then

$$n(x) = \begin{cases} a\exp(\lambda_- x) & \text{for } x > x_2 \\ n_3 + b\exp(\lambda_+ x) + c\exp(\lambda_- x) & \text{for } x < x_2, \end{cases} \tag{21}$$

with $\lambda_\pm = (-v \pm \sqrt{v^2 + 4D\gamma})/2D$. Again, the boundary condition at $x = 0$ and the continuity of $n(x)$ and its derivative at $x = x_2$ determine the constants a, b, and c as functions of x_2. This coordinate is then obtained from $n(x_2) = n_2$. For some special values of $\lambda_\pm$ this calculation can be carried out analytically. A linear stability analysis indicates that this solution is stable.

In Fig. 4, curve 2 corresponds to the solution given by Eq. (21) for $D = 1$, $\gamma = 1$, $v = 1$, $n_3 = 1$, and $x_2 = 3$, which corresponds to $n_2 \approx 0.29$. As discussed in Sec. IV, a constant velocity field is generally not able to stabilize a shock front and stable structures can exist only by the action of an alternative mechanism of density circulation between the diluted and the condensed phases. The curve shown in Fig. 4 is a typical example of a stable structure in these conditions, exhibiting a high population at the nucleation center (compare with Fig. 3).

A third case in which the stationary RDC equation can be exactly solved corresponds to $v(x) = -D_0(x + x_0)^{-1}$, with $D_0, x_0 > 0$, i.e., an implosive decreasing velocity field. According to Eq. (13), this gives rise to an acceptable nucleation pattern, as the density decays as the product of an exponential times a negative power of x. In this case, Eq. (4) becomes

$$0 = (x + x_0)^2 Dn'' + (x + x_0)D_0 n' - \left[D_0 + \gamma(x + x_0)^2\right] n \tag{22}$$

in the diluted region. Defining $n(x) \equiv z^{1-\nu}H(z)$, with $z = \sqrt{\gamma/D}(x + x_0)$ and $\nu = (1 + D_0/D)/2$, Eq. (22) reduces to a modified Bessel equation for $H(z)$ [15]. Therefore, for $x > x_2$, we have

$$n(x) = a(x+x_0)^{1-\nu} K_\nu(\sqrt{\gamma/D}(x+x_0)), \quad (23)$$

where $K_\nu(z)$ is the modified Bessel function with the proper asymptotic behavior. In fact, the large-x dependence of $n(x)$ coincides with Eq. (13).

In the condensed region the mathematical problem becomes more complex. The corresponding Bessel equation presents now a constant inhomogeneity and the general solution must be given in terms of Lommel functions [16]. These can in turn be expressed in integral form, which is more convenient for the numerical evaluation of the solution. For $x < x_2$, the density is

$$\begin{aligned} n(x) = &(x+x_0)^{1-\nu}[bI_\nu(\sqrt{\gamma/D}(x+x_0)) \\ &+cK_\nu(\sqrt{\gamma/D}(x+x_0))] \\ &-(x+x_0)\int_0^{\pi/2} \sinh\left[(x+x_0)\cos\theta\right](\sin\theta)^{2\nu} d\theta. \end{aligned} \quad (24)$$

As in the previous instances, the coefficients a, b, and c in Eqs. (23) and (24) are obtained from the boundary condition at $x = 0$ and continuity requirements at $x = x_2$.

Curve 3 in Fig. 4 corresponds to this solution for $\gamma = 1$, $D = 1$, $\nu = 0.75$, $x_0 = 1$, and $x_2 = 7$, which gives $n_2 \approx 0.48$. In a pure RD system, this value of n_2 would produce an outgoing shock front, so that the condensed region would grow indefinitely and the density would finally approach n_3 for all x. In the presence of convection, the stationary density profile presents a spike at $x = 0$, due to the finite value of $v(x)$ at that point, and, for larger values of x, it is also step shaped. Now, according to the discussion in Sec. IV, we know that the decreasing implosive velocity field we are considering here would not be able to stabilize such a structure, at least for high values of x_2. In fact, a numerical linear stability analysis of this solution shows that it is unstable. This nucleation pattern will then grow and the shock front will eventually reach a region in which the effect of the convection field is negligible.

VI. CONCLUSION

In this paper we have analyzed some aspects of the effect of convective transport on the evolution of reaction-diffusion systems. In particular, we focused attention on the existence and stability of stationary spatial patterns representing nucleation structures, in the frame of bistable reaction models. It is well known that unbounded diffusion cannot stabilize the growth or shrinkage of density domains as, for instance, in phase transitions. Therefore, the question of whether a convective velocity field superposed to diffusion is able to produce a stable localized pattern arises quite naturally.

In order to simplify the mathematical problem we considered a one-species system evolving in one dimension and submitted to diffusive, convective, and bistable reactive processes. We stress that the type of analysis used here to study one-dimensional flows can be easily extended to many-dimensional problems, which, due to suitable symmetries, are described by only one variable. This applies not only to two- or three-dimensional flows with planar symmetry but also, for instance, to radially symmetric cylindrical or spherical systems. In the case of curvilinear coordinates, however, the differential operators in Eq. (4) should be conveniently modified. Certainly, an extremely interesting generalization of our analysis would be to consider flows with many spatial variables. In this case, velocity fields can be much more complex than in one dimension, giving rise to a wide class of new effects, such as distortion of the nucleation centers. This generalization, however, would imply a considerable complication of the mathematical problem and should be treated separately.

Nucleation patterns were characterized as localized structures with a well defined particle number, i.e., with integrable density. In the central or condensed region, which was taken to be symmetric in shape, the density has a relatively high value, usually near the highest stable state of the reaction process. Outside that region, the density must decay rapidly enough to ensure integrability.

It can be easily seen that implosive velocity fields superposed to diffusive transport can produce stationary density structures. Therefore, the question addressed in this paper can be reformulated by asking about the effect of reactions on the evolution of a diffusive and convective species. Here it has been shown that reactions favor the existence of nucleation patterns. In fact, except for some marginal case, they usually determine the diluted-region density to decay exponentially. Hence localized stationary structures associated with nucleation processes in reaction-diffusion-convection systems exist under fairly general conditions.

Determining if such stationary structures are stable is a more difficult task. Usually, a stability analysis requires knowing the explicit form of the solution. This restricts the treatment of our problem to the use of numerical techniques. Numerical simulations of the evolution of the reaction-diffusion-convection system show that, in a broad class of situations, the stability of nucleation patterns depends on the competition of the convective transport and the shock fronts that emerge from the interplay of diffusion and bistable reactions. Roughly speaking, we can say that the velocity field is simply superposed to the shock-front motion. Then, convection will be able to stop the shock front if, at a certain point, the velocity equals in modulus and is opposite in sign to the shock-front speed.

When the initial evolution does not give rise to a shock front, as it usually occurs for shrinking, initially small condensed regions, a different mechanism can nevertheless produce stable patterns for implosive velocity fields. In this situation, a high concentration develops at the nucleation center. Both reaction and diffusion tend to deplete such overpopulation but convection feeds back the center, carrying particles from the diluted region. Eventually, a stable density circulation is established and the nucleation center becomes stationary.

We stress that a more rigorous, global stability analysis could be carried out if it were possible to find a Lyapunov functional for the evolution of the reaction-diffusion-convection system [1,17]. Unfortunately, the dissipative character of the convective term in Eq. (3), which otherwise could be treated through a mechanical analogy [4], makes it difficult to determine the appropriate functional.

Finally, we have presented some exact stationary solutions for various representative forms of the velocity field, in the frame of the Ballast model. This piecewise linearized reaction model preserves, on one hand, the main features of nonlinear bistable models; on the other, its linear character makes its analytical treatment possible. For these stationary solutions, stability can be explicitly studied. In this way, we have verified, at least, in some particular cases, the main conclusions on the stabilization of nucleation patterns by convective transport. Besides the interest of these results in terms of specific problems associated with nucleation processes they are intended to contribute to our understanding on the interplay of reaction, diffusion, and other, more complex transport mechanisms.

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