Effect of partially reflecting boundary conditions on the decay of metastable rest states in an activator-inhibitor system

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We study the effect of the boundary conditions on the spontaneous nucleation and evaporation of excited domains in the bistable regime of an activator-inhibitor stochastic system. In such a regime a *quasivariational* approximation can be used to obtain the stationary distribution. The nucleation and evaporation rates of the resulting nonuniform structures are investigated using a piecewise-linear dynamics to obtain analytical results. [S1063-651X(97)01704-2]

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I. INTRODUCTION

The decay of metastable states (toward globally stable ones) is a recurrent problem in various fields of physics and physical chemistry [1–3]. Typical examples of different nucleation phenomena can be observed even in open systems far from equilibrium [3–7]. The decay of metastable states has been studied for many years, from experimental and theoretical points of view [8,9]. The statistical-mechanical theory was first formulated by Kramers [1], and extended since by several authors. A recent review shows the state of the art [3]. In *reaction-diffusion* (RD) systems, such phenomena can, in principle, be studied in two different ways. The first one is to evaluate the *mean-first-passage–time* (MFPT) between metastable and stable states, and the second one is to find the nucleation rate using the *flux-over-population* (FOP) method. These two procedures are deeply related, and give information on the dynamical response of the system under the effect of fluctuations [3].

Both the MFPT and FOP methods require a knowledge of the stationary probability density. It is a nontrivial task to determine this density in nonvariational RD systems. These situations call for approximations to find out the global distribution. For instance, a WKB-type method has been used to obtain stationary probability densities for some weak-noise cases, conducting (in leading exponential order in the noise strength) to nonequilibrium generalized potentials [10,11].

The features of this phenomenon in spatially extended systems are still under study, particularly when the effect of the boundary conditions (b.c.) is considered. Recently, it has been shown that b.c. play a relevant role in the appearance and stability, as well as on the propagation of spatial structures [12–18]. The nature of the interactions between chemical systems and their environment is a relevant ingredient in the process of establishing a nonequilibrium (dissipative) regime. Particularly, the role that b.c. will play in a chemical reaction will depend on their nature. As an example, the first unambiguous experimental observation of a Turing structure was made in single-phase open reactors for which the systems are fed by diffusion from the boundaries [19]. Here we are concerned with partially reflecting b.c. (*albedo* b.c.), that relate at the boundary Γ the field $u(x,t)$ with its derivative, by an albedo parameter k:

$$\left.\frac{\partial u}{\partial n}\right|_{\Gamma} = \left. -ku(x,t)\right|_{\Gamma} . \tag{1}$$

For one-component bistable RD systems, the change in the relative stability of locally stable attractors induced by a change in the reflectivity of the boundary, was reported in Ref. [14]. These results were extended in Refs. [15,16] to consider the effect of an external noise in the transition between the attractors.

The purpose of this paper is to extend the forementioned analysis to more general bistable systems without the restriction of a variational formulation. We shall concentrate here on a simple model of an *activator-inhibitor* RD system that is *nonvariational*, and investigate the rate of domain formation out of the metastable state, induced by an additive external noise (fluctuations), under the effect of partially reflecting boundary conditions. By a ''quasivariational approximation,'' that is consistent with a singular perturbation approximation, we shall estimate the *nonequilibrium potential* for the system (for stationary patterns), identify the globally stable stationary solution from the metastables ones, and investigate the effect of fluctuations in the spirit of the *flux-over-population* approach to the reaction–rate theory for extended systems.

In the following sections we present a deterministic and a stochastic analysis of the specific model we will work on. First we solve the stationary case with albedo b.c. The study includes a linear stability analysis of the resulting patterns and the calculation of the ''effective nonequilibrium potential'' for the stationary case by using an *quasivariational approximation.*

The stochastic analysis consists in the study of the effect of external additive noises, by focusing on the nucleation

rate of the nonuniform resulting structures and the related MFPT. Section VI includes a final discussion of our results.

II. MODEL

We consider here a simple two-component, excitable RD system, defined in one dimension as:

$$\frac{\partial u(x,t)}{\partial t}=(\epsilon\tau_r)^{(-1)}\left\{\epsilon^2\frac{\partial^2 u}{\partial x^2}+u(1-u)(u-a)-v\right\}$$

$$\frac{\partial v(x,t)}{\partial t}=\frac{\partial^2 v}{\partial x^2}+\beta u-\gamma v, \tag{2}$$

where $u(x,t)$ and $v(x,t)$ are called the activator and the inhibitor, respectively, in a biological context. The constants $\epsilon,\tau_r,\beta,\gamma$, and a are all positive.

The nonlinear nature of Eq. (2) makes these equations difficult to solve, even in the stationary case. We consider the following piecewise-linear version of Eqs. (2) that, while keeping the essential features of the bistable problem, is amenable for analytical calculations:

$$\frac{\partial u(x,t)}{\partial t}=(\epsilon\tau_r)^{(-1)}\left\{\epsilon^2\frac{\partial^2 u}{\partial x^2}-u+\theta[u-a]-v\right\},$$

$$\frac{\partial v(x,t)}{\partial t}=\frac{\partial^2 v}{\partial x^2}+\beta u-\gamma v. \tag{3}$$

Here $\theta[x]$ is the Heaviside step function, and a (>0) is the excitability threshold. Equations (2) and (3) represent a bistable system if $a<\gamma/(\beta+\gamma)$. Otherwise, Eqs. (2) and (3) represent a monostable excitable RD system. This model is a piecewise-linear version of the Bonhoffer–van der Pol system, which is a fundamental model of an excitable RD system [13,17,20]. Such an equation has been used to model the Belousov-Zhabotinskii reaction in the excitable regime [21], pulse propagation in nerve fiber [22,23], the formation of spatial structures in electric glow discharges, etc. [24–27]. For this kind of system, stationary patterns have been predicted in theory and observed in experiments [24,28–30].

As far as a is positive, the piecewise-linear dynamics is essentially the same as the original one. We must emphasize here that neither the original set of equations (2) nor its piecewise-linear version (3) are variational as far as β is positive, because the conditions needed to define a potential are not fulfilled [10]. When the inhibitor field v follows the activator *adiabatically* (that is, when $\epsilon\tau_r\to\infty$), we can consider that $\partial v/\partial t=0$. Here v can be exactly obtained from u, and it is possible to write out a Lyapunov functional for this case. The resulting time-evolution equation for the activator field is nonlocal in the space coordinate [17,31,32].

III. PATTERN FORMATION

In this section, we will solve Eq. (3) with symmetric albedo b.c. for the stationary case. The analysis of stationary-pattern formation for the proposed model, for infinite geometry, was done by Kuramoto [28]. The generalization of the method to finite geometry results straightforwardly [13]. The stationary solution is written as a linear combination of exponentials $\exp(k_i x)$, where k_i are the roots of the characteristic polynomial. The solution is piecewise analytic, with matching points at $|x|=x_c$, where $u(x_c)=a$. The coefficients are fixed by the boundary conditions at $x=\pm L$:

$$\left.\frac{\partial u}{\partial n}\right|_{\pm L}=\left.\mp k u(x,t)\right|_{\pm L},$$

$$\left.\frac{\partial v}{\partial n}\right|_{\pm L}=\left.\mp k v(x,t)\right|_{\pm L}, \tag{4}$$

and the matching conditions at x_c. The stationary solutions are independent of τ_r, since it is a dynamical parameter that specifies the ratio between the relaxation constant of u and that of v.

We will concentrate on simple symmetric patterns. The solution under consideration is such that a central part of the system forms a frozen activated region. The structures have an inner region where u varies abruptly, and two outer regions where the activator and inhibitor fields vary in a smooth fashion. When the parameter ϵ is small enough, these regions are separated by a sharp interface. The albedo boundary conditions will affect the extension of the frozen activated region.

In Fig. 1(a) we show the behavior of the matching coordinate x_c as a function of k for different values of the threshold parameter a. We found that there is a parameter regime (small a) where there are two disconnected branches of x_c, and therefore two nonuniform structures exist that are associated with these parameters. As a increases, a qualitative change in $x_c(k,a)$ occurs. There is a critical value of a, indicated by a_c, such that for $a>a_c$ the two branches coalesce. This last aspect is depicted in Fig. 1(b), for the case of $k\to\infty$ (i.e., Dirichlet b.c.).

It is worth remarking here that, for small enough values of k, there are nonhomogeneous solutions that tend toward the known stable homogeneous Neumann $(k\to 0)$ solutions [13]. However, they are not included in Fig. 1 because in that case the whole pattern is above the threshold a; i.e., it does not have the form we analyze here.

For both open or closed curves, as previously indicated, patterns corresponding to the upper branches have a larger activated zone. It is stability that selects between these branches. Figure 2 shows typical patterns associated to $\epsilon=0.05, a=0.1243, k=4.06$, and $z_L=5$, respectively.

The linear stability results show that the structures that correspond to the upper (lower) branches are stable (unstable). The stable patterns are associated with the existence of an important activated region, which is equivalent to large dissipation. The set of points in the plane (x_c,k) where the two branches coalesce (for $a<a_c$) constitutes the *marginal stability line* that separates stable from unstable behavior [13].

IV. NONEQUILIBRIUM POTENTIAL: QUASIVARIATIONAL APPROXIMATION FOR STATIONARY SOLUTIONS

For the nonuniform stationary patterns associated with the case $\epsilon\ll 1$, a ''quasivariational'' approximation is available,

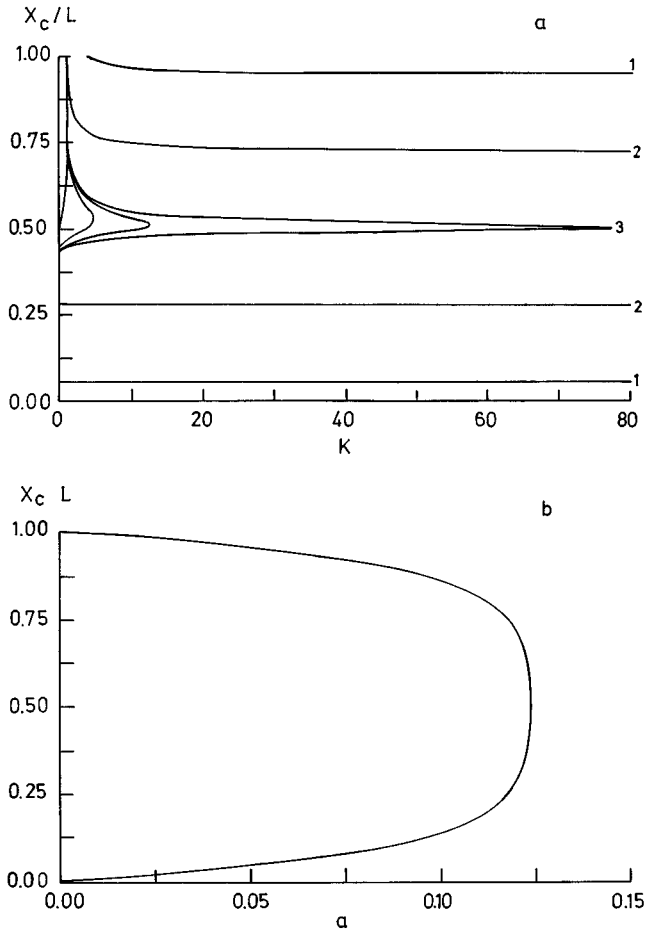

FIG. 1. (a) Values of the matching coordinate x_c as a function of the (dimensionless) albedo parameter k, for a fixed length ($L=5$) and several values of the threshold parameter a: (1) 0.06, (2) 0.12, (3) 0.124 245, (4) 0.1243, (5) 0.1244, and (6) 0.125. (b) Values of the matching coordinate x_c as a function of the threshold parameter a, for $k\to\infty$ (i.e., Dirichlet b.c.). In both cases: $\epsilon=0.05, \beta=1$, and $\gamma=1/3$.

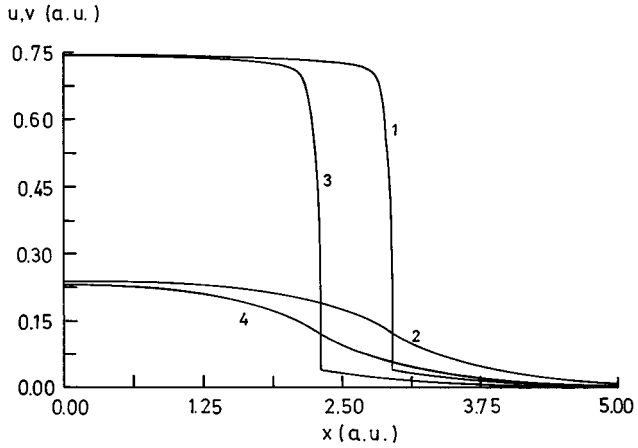

FIG. 2. Typical nonuniform stationary patterns for the activator (u) and inhibitor (v) fields, for the values of the parameters: $k=4.06$, $\epsilon=0.05$, $a=0.1243$, $\gamma=\frac{1}{3}$, and $\beta=1$. The patterns labeled with 1 (activator field) and 2 (inhibitor field) correspond to matching coordinate $x_c=2.9115$ (locally stable), and the patterns labeled with 3 and 4 correspond to activator and inhibitor fields associated to the matching coordinate $x_c=2.3425$ (unstable).

that allows us to identify the globally stable stationary solution of Eq. (2). Following Ref. [5], where such a method was developed, we divide the functional space into two parts. One is the shape of $\{u\}$ in the *inner* region of the interface, where we exploit the fact that the variation of the field v is not significant. The nonequilibrium potential in this region as is approximated:

$$\mathcal{L}_{\text{inner}}\{u(x),v(x)\sim v_I\}=\frac{1}{\epsilon\tau_r}\int_{X_c-\epsilon}^{X_c+\epsilon}dx\left\{\frac{\epsilon^2}{2}\left(\frac{du}{dx}\right)^2+\frac{u^2}{2}+v_I u-(u-a)\,\theta[u-a]\right\}, \tag{5}$$

where v_I is a characteristic value of the inhibitor field in the inner region [in our calculation, $v_I=v(x_c)$]. The integration domain is limited to the region where $|x_c|-\epsilon\leqslant|x|\leqslant|x_c|+\epsilon$.

On the other hand, in the outer regions we approximate the stationary behavior of the activator by considering that $\epsilon\sim 0$ (this approximation is consistent with the singular perturbation method [20]). For that case $v=-u+\theta[u-a]\to u=h^{\pm}(v)$, and the nonequilibrium potential in these regions results in:

$$\mathcal{L}_{\text{outer}}\{u(x)\sim h^{\pm}(v),v(x)\}=\int_{\text{out}^{\pm}}dx\left\{\frac{1}{2}\left(\frac{dv}{dx}\right)^2+\frac{1+\gamma}{2}v^2+(v_I-v)\,\theta[|x|-x_c]\right\}+\frac{k}{2}v^2\Big|_L+\frac{k}{2}v^2\Big|_{-L}, \tag{6}$$

where the integration domains are limited to the regions $|x|\leqslant|x_c|-\epsilon$ for the out$^+$ region and $|x_c|+\epsilon\leqslant|x|\leqslant L$ for the out$^-$ region, respectively.

The nonequilibrium potential for Eq. (3) can be approximated, *for the stationary case*, as

$$\mathcal{L}_{\text{NE}}=\mathcal{L}_{\text{outer}^+}+\mathcal{L}_{\text{outer}^-}+\mathcal{L}_{\text{inner}}. \tag{7}$$

The (locally stable) uniform state $u=v=0$ (that lies on the thermodynamical branch) can also be included in Eq. (7). As the averages of u,v, and v_I are zero at this uniform state, this results in:

$$\mathcal{L}_{\text{NE}}\{u=0,v=0\}=0. \tag{8}$$

In Figs. 3 and 4 we show the numerical value of $\mathcal{L}_{\text{NE}}$ as a function of k for several values of a. In Fig. 3, the lower (upper) branches correspond to the larger (smaller) values of x_c, corresponding to the metastable (unstable) nonuniform stationary patterns. In Fig. 4 we show the behavior of the nonequilibrium potential for small values of a. We conclude that for this parametric regime, the nonhomogeneous stationary solutions associated with the upper branches in Fig. 1(a) are the *globally stable solutions*. This situation *changes* when the threshold increases, as can be inferred from Fig. 3, resulting in a *change in the relative stability* between the nonuniform patterns and the homogeneous solution

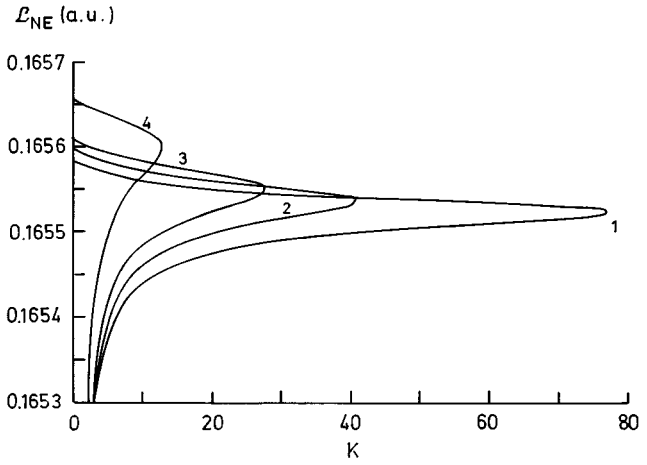

FIG. 3. Values of the nonequilibrium potential $\mathcal{L}_{\rm NE}$ as a function of the (dimensionless) albedo parameter k, corresponding to cases between curves (3) and (4) in Fig. 1: the values for the threshold parameter a are (1) 0.124 245, (2) 0.124 255, (3) 0.124 265, and (4) 0.1243. The upper (lower) branches corresponds to the lower (upper) closed branches in Fig. 1, and they are associated with the unstable (metastable) nonuniform patterns. Here we have used $\epsilon=0.005$, $\epsilon\tau_r=10$, $\beta=1$, $\gamma=\frac{1}{3}$, and $L=5$.

$(u=0,v=0)$. The upper branches in Figs. 3 and 4 correspond to the unstable solutions and represent the barrier between the uniform and nonuniform locally stable solutions [14,15]. If we consider that $\mathcal{L}_{\rm NE}\{u=0,v=0\}=0$, these upper branches give themselves the magnitude of the barrier when the uniform state $u=v=0$ represents the metastable phase (as in Fig. 4). It is worth remarking here that, as can be inferred from Fig. 1(b), the upper and lower branches in Fig. 4 will not join, even in the limit $k\to\infty$.

When $x_c\to L$ the approximation fails because the nonuniform patterns experience a qualitative change in their profiles (the size of the activated region results of the order of L).

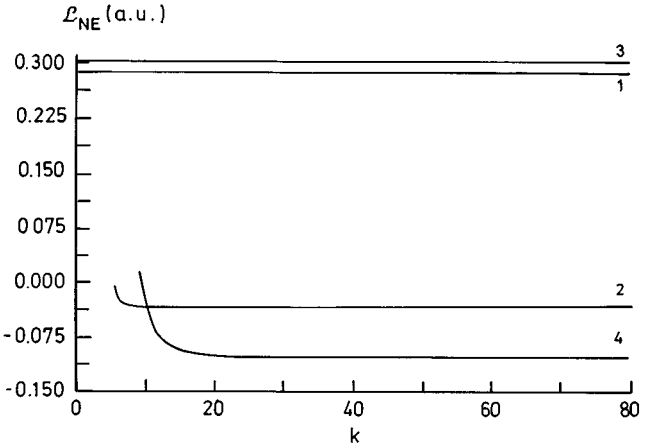

FIG. 4. Values of the nonequilibrium potential $\mathcal{L}_{\rm NE}$ as a function of the (dimensionless) albedo parameter k, corresponding to the case of open branches in Fig. 1. Here $\epsilon=0.005$, $\epsilon\tau_r=10$, $\beta=1$, $\gamma=\frac{1}{3}$, and $L=5$. For (1) and (2), the value of the threshold parameter was $a=0.04$; while, for (3) and (4), it was $a=0.06$. The upper branches 1 and 3 correspond, for all values of k, to the unstable nonuniform patterns.

For this case the approximation cannot be applied, and the value of $\mathcal{L}_{\rm NE}$ loses its meaning. This fact explains why the lower branch increases abruptly for small enough values of k.

V. NUCLEATION RATE

In Sec. IV, we showed that the behavior of the nonvariational system [Eqs. (2) and (3)] is quasipotential when the limit $\epsilon\ll 1$ is considered. Here the nucleation rate of nonhomogeneous structures is calculated using the flux-overpopulation method [3]. For the sake of completeness, here we repeat some steps of the procedures developed in Ref. [5]. We consider Eq. (3) with independent additive external noises $f_i(x,t)$,

$$\frac{\partial u(x,t)}{\partial t}=(\epsilon\tau_r)^{(-1)}\left\{\epsilon^2\frac{\partial^2 u}{\partial x^2}-u+\theta[u-a]-v\right\}+f_1(x,t)$$

$$\frac{\partial v(x,t)}{\partial t}=\frac{\partial^2 v}{\partial x^2}+\beta u-\gamma v+f_2(x,t). \tag{9}$$

$f_i(x,t)$ are chosen as Gaussian and white,

$$\langle f_i(x,t)\rangle=0,$$

$$\langle f_i(x,t),f_j(x',t')\rangle=2\delta_{ij}g_i\delta(t-t')\delta(x-x'), \tag{10}$$

where $i,j=1,2$, and g_i is the noise intensity. This noise affects the system in an additive manner:

$$\frac{\partial u_i}{\partial t}=F_i\{u\}+f_i. \tag{11}$$

Equation (11) assumes that the space has been discretized into a regular lattice, so that u_i and f_i are defined at the lattice points i, and $F_i\{u\}$ are the sum of the (local) reaction terms plus the spatially discretized version of the diffusion term. The subscript i labels both the lattice point and the chemical species, so that $\Sigma_i u_i=\Sigma_{j=1,2}\int_{-L}^{L}u_j(x)dx$, where $u_1=u$ and $u_2=v$. Equations (9) and (10) can be transformed into a Fokker–Planck equation for the probability density $P\{u_i,t\}$,

$$\frac{\partial P}{\partial t}\{u_i,t\}=\left[\sum_{ij}g_{ij}\frac{\partial^2}{\partial u_i\partial u_j}-\frac{\partial F_i}{\partial u_i}\right]P\{u_i,t\}, \tag{12}$$

where $g_{ij}=g_i\delta_{ij}$ [the discrete version of $g_i\delta(x-x')$]. The stationary distribution is readily obtained using the nonequilibrium potential

$$P_o\{u\}=C\exp[-\mathcal{L}_{\rm NE}\{u\}/g], \tag{13}$$

where C is the normalization constant. Equation (13) represents the global distribution for Eq. (12). For simplicity we have fixed $g_1=g_2=g$.

In the FOP method, the rate at which the metastable state decays is calculated in terms of the ratio of the *total* probability flux crossing the energy barrier and the population of the *metastable state* corresponding to a stationary current-

carrying situation [3,5]. To obtain it, we first need the stationary distribution *around the saddle point* $u^{(s)}$. Linearizing F around this unstable state,

$$F_i=\sum_j A_{ij}v_j$$

$$v_i=u_i-u_i^{(s)}, \tag{14}$$

we obtain

$$P^{(s)}\{v\}=C_s\exp\left[-\frac{1}{2}\sum_{ij} s_{ij}v_iv_j\right], \tag{15}$$

and C_s is a positive constant: $C_s=\exp[-\mathcal{L}\{u_s\}]$. By an orthogonal transformation M that diagonalizes the variance $\sigma_{ij}=(s^{-1})_{ij}$, the resulting stationary distribution can be written in terms of $\xi_i=\Sigma_j M_{ij}v_j$ as [3,33]

$$P^s\{\xi\}=C_s\exp\left[-\frac{1}{2}\sum_j \frac{\xi_j^2}{\sigma_j}\right]. \tag{16}$$

The other matrices are also transformed in the form $\|\widetilde{A}\|=\|M\|\|A\|\|M^T\|$. We choose σ_1 as the *negative* variance associated with the *unstable* mode. We have calculated the probability current that flows from the locally stable (metastable) uniform pattern to the more stable nonuniform pattern. The steady current $\widetilde{J}_n$ is defined by

$$\widetilde{J}_n\{\xi\}=-\left[\sum_m \widetilde{g}_{mn}\frac{\partial}{\partial\xi_m}-\widetilde{F}_n\right]P\{\xi\}, \tag{17}$$

which satisfies

$$\sum_n \frac{\partial\widetilde{J}_n}{\partial\xi_n}=0. \tag{18}$$

In the flux-over-population method, boundary conditions in functional space are imposed so that there is a source of the current at the metastable state and a sink at the stable solution [3]. Therefore, the magnitude of the current near the saddle point is *stationary*.

The usual ansatz to solve Eq. (18) is

$$P\{\xi\}=\rho\{\xi\}P_s\{\xi\}, \tag{19}$$

where $P_s\{\xi\}$ is the stationary distribution of Eq. (12) without either sink or source. Near the saddle point (where there are no sources or sinks), we can use the linearized form (14) and (15) with $P_s\{\xi\}=P^s\{\xi\}$, resulting in:

$$\sum_{mn}\left[\widetilde{g}_{nm}\frac{\partial^2}{\partial\xi_n\partial\xi_m}+\widetilde{A}_{nm}\frac{\sigma_n}{\sigma_m}\xi_m\frac{\partial}{\partial\xi_m}\right]\rho\{\xi\}=0. \tag{20}$$

To solve Eq. (18), we assume that

$$\rho\{\xi\}=\phi(y), \tag{21}$$

as in Ref. [5], where y is linear in the deviation from the saddle-point,

$$y=\sum_n U_n\xi_n. \tag{22}$$

Equation (20) is now written as,

$$\gamma\frac{d^2\phi}{dy^2}-y\frac{d\phi}{dy}=0, \tag{23}$$

where

$$\kappa^{-1}\sum_{mn} U_m\widetilde{g}_{mn}U_n=\gamma, \tag{24}$$

κ being the rate of growth of the unstable mode at the saddle point [3,33] (the positive eigenvalue of the matrix $||\widetilde{A}||$). The formal solution to Eq. (23) that already satisfies the boundary conditions is given by

$$\phi(y)=\frac{C'}{\sqrt{2\pi|\gamma|}}\int_y^\infty dy'\exp\left[\frac{y'^2}{2\gamma}\right], \tag{25}$$

with C' a constant. The nontrivial solution is acceptable only if γ is negative, in which case $\phi(y)$ is an error function. The constant C' can be calculated by normalizing $P\{u\}$ in the metastable region: we approximate $P_s\{u\}$ by a Gaussian distribution around the metastable state $u^{(m)}$,

$$P_s\{u\}=\exp\left[-\mathcal{L}_{\rm NE}^{(m)}/g+\sum_{ij} B_{ij}\eta_i\eta_j\right], \tag{26}$$

where $\mathcal{L}_{\rm NE}^{(m)}(=\mathcal{L}_{\rm NE}\{u^m\})$ is calculated from the global distribution, and $\eta_i=u_i-u_i^{(m)}$ Using Eqs. (19), (25), and (26), we determine the constant

$$(C')^{-1}=\int d\{\eta\}P_s\{\eta\}=\exp[-\mathcal{L}_{\rm NE}^{(m)}/g]\left(\prod_n \sqrt{(2\pi\sigma_n^{(m)})}\right), \tag{27}$$

where $\sigma_n^{(m)}$ are the eigenvalues of $||B^{-1}||$ in Eq. (26). The resulting current is

$$J_n=|\kappa|\sigma_nU_nP^{(s)}\{\xi\}\frac{d\phi}{dy}. \tag{28}$$

To obtain the nucleation rate, we must calculate the probability current that flows across the surface $\xi_1=0$ of the unstable mode [33],

$$I=\int_{\xi_1=0}d\{\xi\}J_1=|\kappa|\sigma_1U_1\int_{\xi_1=0}d\{\xi\}P^{(s)}\{\xi\}\frac{d\rho}{dy}. \tag{29}$$

We finally obtain the nucleation rate I as:

$$I=\left(\frac{|\sigma_1|}{2\pi}\right)^{1/2}|\kappa|\left(\prod_n{}'\sqrt{2\pi\sigma_n}\right)\left(\prod_n \sqrt{2\pi\sigma_n^{(m)}}\right)^{-1}$$
$$\times\exp(-[\mathcal{L}_{\rm NE}^{(m)}-\mathcal{L}_{\rm NE}^{(s)}]/g), \tag{30}$$

where $\mathcal{L}_{\rm NE}^{(s)}=\mathcal{L}_{\rm NE}\{u^{(s)}\}$ and the prime in Π' means that the unstable mode σ_1 is excluded. The negative variance σ_1 is related with κ, and σ_1 is simply given by [5]

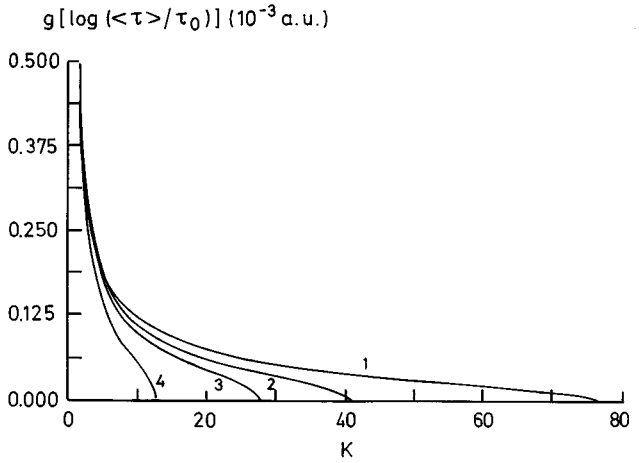

FIG. 5. Values of $g\log_{10}(\langle\tau\rangle/\tau_0)$ as a function of the (dimensionless) albedo parameter k, for a fixed length $L=5$, and the following values of the threshold parameter a: (1) 0.124 245, (2) 0.124 255, (3) 0.124 265, and (4) 0.1243. Here $\beta=1$, $\gamma=\frac{1}{3}$, $\epsilon=0.05$, and $\epsilon\tau_r=10$. $\langle\tau\rangle$ denotes the MFPT associated with the evaporation of nonuniform structures.

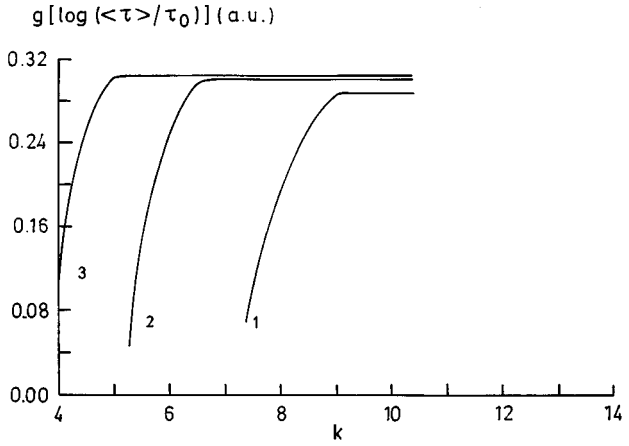

FIG. 6. Values of $g\log_{10}(\langle\tau\rangle/\tau_0)$ as a function of the (dimensionless) albedo parameter k, for a fixed length $L=5$ and the following (small) values of the threshold parameter a: (1) 0.04, (2) 0.05, and (3) 0.06. Here $\beta=1$, $\gamma=\frac{1}{3}$, $\epsilon=0.05$, and $\epsilon\tau_r=10$. $\langle\tau\rangle$ denotes the MFPT associated with the transition between metastable and stable states. The constant region of the curves corresponds to the nucleation of nonuniform structures.

$$\sigma_1=g/\kappa. \tag{31}$$

With the global steady distribution, we can obtain $[\mathcal{L}_{\rm NE}^{(m)}-\mathcal{L}_{\rm NE}^{(s)}]$. The effect of the boundary conditions appears essentially in $\mathcal{L}_{\rm NE}$. A similar result (in a monostable regime) was obtained by Ohta in Ref. [5] for infinite geometry.

If there is a reasonable separation of time scales, the mean-first-passage time is simply determined by half the inverse of the nucleation rate:

$$\langle\tau\rangle=\tau_0\exp(-[\mathcal{L}_{\rm NE}^{(s)}-\mathcal{L}_{\rm NE}^{(m)}]/g). \tag{32}$$

The factor τ_0 is usually determined by the curvature of $\mathcal{L}_{\rm NE}$, and is typically several orders of magnitude smaller compared to the average time $\langle\tau\rangle$ [3,5]. The prefactor is expected not to produce any singular behavior except near the marginal stability line [where $\mathrm{Re}(\kappa)\to 0$]. In this region, the unstable state *is not well isolated* [15,18], and the whole approximation fails, since it has been derived under the assumption that the saddle point is well separated from the stable nonuniform state. Near the marginal stability line, the nucleation rate (30) is only *qualitatively* valid; nonetheless, the growth rate itself is meaningful [5].

The behavior of $\langle\tau\rangle$ (or more properly of $g\ln(\langle\tau\rangle/\tau_0)$ as a function of the albedo parameter k is shown in Fig. 5 for the case where the globally stable stationary state is the uniform solution $u=v=0$. Here $\langle\tau\rangle$ is associated with the process of *evaporation* of nonuniform metastable patterns (it refers to the stability of the homogeneous state).

In Fig. 6 we show the behavior of the MFPT between metastable and stable states for the small-a parametric regime. In the region, where the homogeneous solution is the globally stable one, $\langle\tau\rangle$ (the MFPT associated to the evaporation of metastable nonuniform patterns) results to be a monotonically increasing function of k, until some $k_{\rm crit}$ (dependent upon a) is reached, for which a *stability exchange* occurs. Above that value, the stable state is now the inhomogeneous one, and τ (the MFPT associated to the process of nucleation of nonuniform patterns) remains constant.

VI. CONCLUSIONS

By applying the method developed in Ref. [5], we explored the influence of a controlled flux at the boundary of the relevant species, for instance chemical, on the self-organizing behavior of a one-dimensional activator-inhibitor system in a bistable regime. The b.c. considered correspond to adjusting the gradient of the concentrations of the fields at the boundaries in proportion to the value of the concentration itself (the albedo parameter represents this ratio). Using a ''quasivariational approximation'' (because our system is *non*variational) we analyze the global stability of the resulting stationary patterns. We have found that the bistable behavior of the system is governed (in the limit $\epsilon<1$) by a *functional* $\mathcal{L}_{\rm NE}$ that approaches the numerical value of the nonequilibrium potential for the relevant states in the nucleation or evaporation processes. The ''effective potential'' here obtained allows us to identify the stable stationary patterns from the metastable ones, as well as the direct calculation of the barrier height between these attractors. A change in the relative global stability between uniform and nonuniform stable stationary states is seen as the threshold increases or the reflectivity of the boundary decreases. A similar behavior was found in a single-component bistable system [14,15,18]. The nucleation rate of inhomogeneities for this system and the evaporation rate of metastable inhomogeneities were calculated by the flux-over-population method, and we used the effective Lyapunov functional to obtain the stationary global probability distribution.

Summarizing, we found that the reflectivity at the boundary alters the local stability properties of the homogeneous stationary solution, producing changes in the basin of the homogeneous attractor. This influence results in a modification of the parameter region of stability for the solutions as

the albedo parameter is varied. The albedo b.c. give a simple way to alter the stability of the thermodynamic branch, and it allows us to advance or retard self-organizing phenomena without altering the nonlinear dynamics of the systems. For systems that admit a nonequilibrium potential it is known that partially reflecting b.c. alter such a potential by adding to it a ''surface term'' [14–16]. We hope that the present analysis will stimulate the experimental search of this kind of phenomenon. Considering the interesting generation of open reactors fed by diffusion from the boundaries, the possibility of controlling the boundary conditions seems to be feasible.

The present ''quasivariational'' approach opens the possibility of studying the decay of metastable states, or (generally speaking) transitions between locally stable states, when the system is subject to external noises, for a large variety of situations of great practical interest. The analysis of such situations will be the subject of further work.

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