Nucleation Rate of a Localized Structure in a Reaction-Diffusion System

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We derive the nucleation rate of a localized structure of a one-dimensional, nonlocal, bistable reaction diffusion equation near instability of the uniform state.

Nucleation and dynamics of localized structures in dissipative, bistable systems described by nonlinear partial differential equations are of great experimental and theoretical interest in the field of pattern formation ([1–5] and refs. therein). In a typical situation the uniform state of a spatially extended system becomes unstable at a critical point in control parameter space, and a new state emerges with finite amplitude in a localized region. Of numerous examples we mention here only the formation of a current filament in SNDC semiconductors [6–7], where a tube or a sheet (which is described by one space dimension) of high current density is formed.

The theoretical description of the symmetry-breaking structure is often based on a reduction of the total function space to a subspace, justified by the existence of some small scales. For example, in systems described by reaction-diffusion equations it is in some cases possible to derive an ordinary differential equation for the diameter of an n-dimensional growing domain if the ratio of wall thickness and diameter is a small quantity.

In the present contribution we are concerned with a simple one-dimensional, nonlocal model. In a certain range of the control parameter μ it exhibits bistability of a uniform and a localized finite-domain state. We derive the nucleation rate of the latter in a defined region below the instability of the former at the subcritical bifurcation of the localized structure. The saddle between the two stable states cannot be reduced to a diameter variable, i.e. it does not have the form of a domain with a sharp front. Therefore the concept of a critical radius becomes meaningless.

Let us consider the partial differential equation for the one-component field $\phi(x, t)$ ($|x| \leq R$):

$$\partial_t \phi = \partial_x^2 \phi + g(\gamma, \mu) - f(\phi) + \xi(x, t). \tag{1}$$

The nonlinear function f is modelled by the piecewise linear function

$$f = \begin{cases} q^{-2}\phi, & \text{if } \phi < 0, \\ -\phi, & \text{if } 0 \leq \phi \leq 1, \\ p^{-2}\phi - (1 + p^{-2}), & \text{if } 1 < \phi. \end{cases} \tag{2}$$

$g(\gamma, \mu)$ depends on the nonlocality

$$\gamma = \frac{1}{2R} \int_{-R}^{R} \phi \, \mathrm{d}x. \tag{3}$$

In the above mentioned example of current-filament formation, the control parameter and the nonlocal quantity are the bias voltage and the current, respectively, entering the partial differential equation for the carrier density through the electric field. ξ is weak white noise defined by $\langle \xi \rangle = 0$ and $\langle \xi(x, t)\, \xi(y, s) \rangle = 2\beta^{-1}\delta(x - y)\,\delta(t - s)$, $\beta \gg 1$. The boundary conditions are $\partial_x \phi(\pm R) = 0$. Further, we assume the diameter of the system to be very large compared to all other length scales of the system: $R \gg \max(p, q, 1)$. From this follows the existence of a translational Goldstone mode of nonuniform stationary solutions (we neglect quantities of the order $\exp(-q^{-1}R)$).

The stationary solutions are the intersections of the curve $g = g(\gamma, \mu)$ with the branches $\gamma = h_i(g)$ in the g–γ-plane (Figure 1). The $h_i(g)$ are obtained by solving (1) for ϕ at fixed g and using (3). Here, we are interested in the uniform solution $\phi_m(x) = \tilde{\phi}_1 = q^2 g$, and in the localized solutions $\phi_l(x)$ with the property $\phi_l(x) \to \tilde{\phi}_1$ if $|x| \gg 1$. The $\phi_l(x)$ exist for $0 > g > g_{eq}$,

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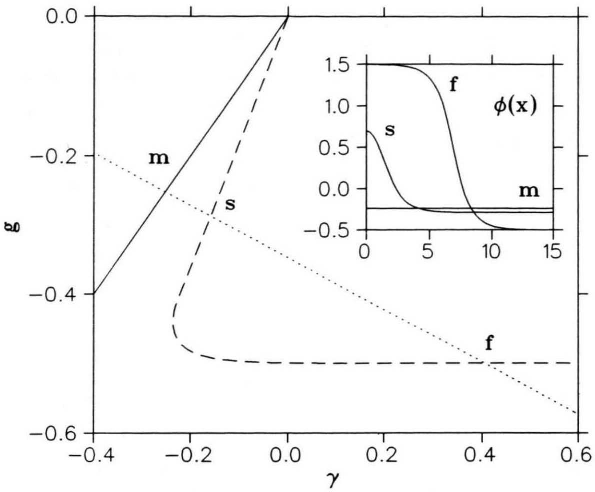

Fig. 1. The stationary solutions of (1) are the intersections of $g=g(\gamma,\mu)$ (dotted line) and the γ–g-characteristics $\gamma=h(g)$ for the uniform (solid line) and the localized state (dashed line). The corresponding functions $\phi(x)$ are shown in the inset ($p=q=1$, $R=15$).

where

$$g_{\mathrm{eq}}=-\left(1+\sqrt{\frac{1+q^2}{1+p^2}}\right)^{-1}. \tag{4}$$

We require $g(\gamma,\mu)$ to guarantee bistability. As an example we take the simple form $g=\mu-\alpha\gamma$, where α is some suitably chosen positive constant. The unstable localized solutions will be labeled by the indices s and f, respectively. For the following, the value of g corresponding to the saddle is restricted to $0>g\geq g_{\mathrm{c}}$, where

$$g_{\mathrm{c}}=-(1+\sqrt{1+q^2})^{-1}. \tag{5}$$

In this region the radius of the localized solution (s) is fixed and the amplitude increases for decreasing g. Below the instability of the uniform state (m) at $\gamma=g=0$, this solution (s) corresponds to a saddle in function space, which has to be jumped over in order to nucleate the stable, localized state (f). We find for the uniform solution $h_{\mathrm{m}}=\tilde{\Phi}_1$, and $h_{\mathrm{s}}(g)=\tilde{\Phi}_1+(\tilde{\Phi}_2-\tilde{\Phi}_1)(x_{\mathrm{a}}+q)\,R^{-1}$. $\tilde{\Phi}_{1,2}(g)$ are the solution of $g=f(\phi)$ for $\phi<0$ and $0\leq\phi\leq1$, respectively, and $x_{\mathrm{a}}=\pi-\arctan(q)$.

An essential property of (1) is the existence of a Lyapunov functional

$$E[\phi]=\int \mathrm{d}x\left(\tfrac{1}{2}(\partial_x\phi)^2+V_1(\phi)\right)+2RV_2\left(\left(\frac{1}{2R}\int\phi\,\mathrm{d}x\right),\mu\right), \tag{6}$$

where $V_1'=f$ and $\partial_\gamma V_2(\gamma,\mu)=-g(\gamma,\mu)$. This allows to derive the nucleation rate r in the framework of classical nucleation theory (see e.g. [8]):

$$r=\frac{\lambda_0^{\mathrm{s}}}{2\pi}\,S\exp(-\beta\Delta E). \tag{7}$$

$\Delta E=E[\phi_{\mathrm{s}}]-E[\phi_{\mathrm{m}}]=(1+q^2)(x_{\mathrm{a}}+q)(1+\alpha q^2)^{-2}\mu^2$ is the activation energy, and the $\lambda_n^{\mathrm{s,m}}$ are the (ordered) eigenvalues of the stability eigenvalue problem. They are given by the zeros of transcendental functions $D^{\mathrm{s,m}}(\lambda)$, similar to well-known eigenvalue problems in quantum mechanics. Clearly, $\lambda_n^{\mathrm{m,s}}<0$, with the exceptions $\lambda_0^{\mathrm{s}}>0$ and $\lambda_1^{\mathrm{s}}=0$, where terms of the order $\exp(-q^{-1}R)$ have been neglected. λ_0^{s} and λ_1^{s} correspond to the unstable mode of the saddle and the Goldstone mode. The functions h_f and $E[\phi_f]$ are not needed in this context.

The remaining part of this note is left to the main problem, namely the derivation of the static prefactor

$$S=2\tilde{R}\sqrt{-\frac{\prod\limits_n(-\lambda_n^{\mathrm{m}}\beta\backslash(2\pi))}{\prod\limits_{n\neq1}(-\lambda_n^{\mathrm{s}}\beta\backslash(2\pi))}} \tag{8}$$

in (7), where $2\tilde{R}=2R\sqrt{\int\mathrm{d}x(\phi_{\mathrm{s}}')^2}$ is the volume of the subspace generated by translation of ϕ_{s} in function space. To this end we use the identity

$$\frac{D^{\mathrm{m}}(\lambda)}{D^{\mathrm{s}}(\lambda)}=\frac{\prod\limits_n(\lambda-\lambda_n^{\mathrm{m}})}{\prod\limits_n(\lambda-\lambda_n^{\mathrm{s}})}, \tag{9}$$

holding for suitably normalized $D^{\mathrm{m,s}}(\lambda)$. To deal with the zero eigenvalue in the denominator of (9), we compute all quantities up to the first nonvanishing order in $\exp(-q^{-1}R)$, multiply (9) at $\lambda=0$ by $\lambda_1^{\mathrm{s}}\beta(2\pi)^{-1}$ and obtain finally

$$S=2R\sqrt{\frac{\beta}{\pi}q\,g_{\mathrm{s}}^2}\sqrt{\frac{1-(\partial_\gamma g\,h'(g))_{\mathrm{m}}}{1-(\partial_\gamma g\,h'(g))_{\mathrm{s}}}}\exp\left(\frac{x_{\mathrm{a}}}{q}\right). \tag{10}$$

To conclude, we mention that in our example, sufficiently near to the instability of the uniform state, the saddle cannot be reduced to a radius variable, even in the limit without nonlocality ($|\alpha|\ll1$), when the stable state ϕ_f is not localized but uniform. Similar results are expected to be valid for higher space dimensions n. The reason is that for $0>g\geq g_{\mathrm{c}}^{(n)}$, the unstable mode of the localized solution is an amplitude mode rather than a radius mode. However, if α is small enough, the reduction to a radius variable becomes very useful in the weakly supersaturated case, and nucleation can be described approximately by stochastic wandering of the wall [2].

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