

Stable Kink-Antikink Pairs in Bistable Reaction-Diffusion Systems with Strong Nonlocalities*

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Z. Naturforsch. **50 a**, 1128–1134 (1995); received August 16, 1995

We investigate the statics, nucleation, and dynamics of stable kink-antikink pairs (KAP) in a one-dimensional, one-component reaction-diffusion equation with a piecewise linear nonlinearity. The stabilization of the KAP is due to the presence of a strongly nonlocal inhibitor. We find a saddle-node bifurcation of a metastable KAP with a separation proportional to $\ln L$, where L is the length of the sample. The KAP becomes globally stable at a characteristic separation proportional to \sqrt{L} . The nucleation of a KAP from the metastable uniform state differs from the case without nonlocality mainly by a change of the activation energy induced by the nonlocality. Furthermore, we investigate the dynamics of the stable KAP in the presence of an external driving force and a diluted density of pointlike impurities; in particular, we derive expressions for the mobility and the average elongation of the KAP.

1. Introduction

Nucleation and dynamics of localized structures are of considerable experimental and theoretical interest in nonlinear dynamics of spatially extended systems driven far from equilibrium (see, e.g., [1]). In this paper, we study the properties of stable kink-antikink pairs (KAP) in a spatially one-dimensional reaction-diffusion system with Neumann boundary conditions. A KAP can be visualized by a domain of finite width of a certain phase connected on either side to another stable phase by domain walls with a thickness related to a characteristic diffusion length. The existence of a stable static KAP is a non-trivial problem. It is well-known that in local reaction-diffusion systems with a one-component order-parameter field there exists an energy functional. As a consequence, there are no stable stationary KAP's in the homogeneous bulk, since a domain wall connecting states with different energy densities always moves towards the high-energy domain in order to lower the energy [2]. Even in the nongeneric case where a domain wall connects different states with the same energy density, it turns out

that a stationary KAP is unstable against variations of the domain width, reflecting the interaction of nonuniform states with each other and with the boundaries of the system. We mention that, however, an unstable static KAP is not meaningless since it represents the critical nucleus for a noise-induced order-parameter change [3].

A nonlocal inhibition can serve as a possible mechanism for the formation of a stable static KAP [4]. In general, *nonlocalities* occur in systems where a fast propagating field has been eliminated by the approximation of an infinite propagation velocity [5]. Typical examples are mean-flow effects in fluid convection [6], localized patterns in biological activator-inhibitor systems with a fast diffusing inhibitor [7], appropriately biased current instabilities [8], and ferromagnetic resonance instabilities [9]. In order to investigate a system with the typical properties of these examples and which is as simple as possible, we choose a bistable reaction-diffusion equation with a strong nonlocality, i.e. where the characteristic nonlocal length scale is larger than the sample length [10].

This paper is organized as follows. In Sect. 2 the model is introduced. The relevant steady states are discussed in Section 3. The nucleation problem is discussed in Section 4. The behavior of the stable KAP under the influence of external forces is studied in Sect. 5, and in Sect. 6 an example corresponding

* Paper presented at the 5th Annual Meeting of ENDADYN, Grenoble, October 10 - 13, 1994.
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to localized impurities and an external force which couples to the translational mode of the KAP is considered.

2. The Model

We consider a system which is described by the following reaction-diffusion equation for a one-component order-parameter field $\phi(x, t)$:

$$\partial_t \phi = \partial_x^2 \phi + g(\bar{\phi}, \mu) - f(\phi) + \varepsilon F[\phi, x, t], \quad (1)$$

where ϕ satisfies homogeneous Neumann boundary conditions, $\partial_x \phi|_{\pm L/2} = 0$. The nonlinearity $f(\phi)$ is modelled by the continuous and piecewise linear function

$$f(\phi) = \begin{cases} f_1 = q^{-2}\phi, & \phi < 0, \\ f_2 = -\phi, & 0 \leq \phi \leq 1, \\ f_3 = p^{-2}\phi - (1 + p^{-2}), & 1 < \phi. \end{cases} \quad (2)$$

In the following we assume that the sample length L is much larger than any other length scale, i.e., $L \gg 1, p, q$. The function

$$g(\bar{\phi}, \mu) = \mu - \alpha \bar{\phi} \quad (3)$$

depends on the control parameter μ and on the order parameter

$$\bar{\phi} = \frac{1}{L} \int_{-L/2}^{L/2} dx \phi, \quad (4)$$

and α is a coupling constant. The functions f and g are shown in the inset of Figure 1. The last term εF in (1) represents small forces ($\varepsilon \ll 1$) due to weak impurities in the sample, external fields, noise etc. To give an example, the formation of current-filaments [8] in one transverse space dimension can be modeled qualitatively by (1) describing the diffusion and the generation-recombination processes of the carrier density ϕ . The coupling to the external circuit is described by the ‘load-line’ $g(\bar{\phi}, \mu)$, where g and μ represent the voltage drop across the sample and the bias voltage, respectively. An external force of the form $F \propto \partial_x \phi$ arises in the presence of a magnetic field [11]. This type of a force will be taken up in Section 6.

An essential property of the dynamic system defined by (1) is the existence of the ‘energy’ functional

$$E[\phi] = \int_{-L/2}^{L/2} dx \left(\frac{1}{2} (\partial_x \phi)^2 + V_1(\phi) \right) + L V_2(\bar{\phi}, \mu) \quad (5)$$

with $V_1'(\phi) = f(\phi)$ and $\partial_{\bar{\phi}} V_2(\bar{\phi}, \mu) = -g(\bar{\phi}, \mu)$. Indeed, one can rewrite Equation (1) in the form $\partial_t \phi = -\delta E[\phi]/\delta \phi + \varepsilon F$, which implies that for $\varepsilon = 0$, time-dependent attractors (as, e.g., limit cycles) do not occur and any solution will approach a stable stationary state since the energy is bounded from below. Furthermore, if εF is associated with white noise, the decay of metastable states can be investigated by the well-known multi-dimensional Kramers theory (see, e.g., [3]).

3. The Stable Steady States

In order to construct stationary solutions it is convenient to solve (1) for ϕ first at fixed g . Once the solution $\phi(x; g)$ is known, one can calculate the spatial average $\bar{\phi}(g)$. The stationary solutions of the nonlocal problem finally correspond to the intersection points of the curves $\bar{\phi} = \bar{\phi}(g)$ and $g = g(\bar{\phi}, \mu)$ in the $\bar{\phi}$ - g plane (self-consistency condition).

One finds from (1) and (2) that the uniform states are given by $\bar{\phi}(g) = \bar{\phi}_1 \equiv q^2 g$ if $g < 0$, $\bar{\phi}(g) = \bar{\phi}_2 \equiv -g$ if $-1 \leq g \leq 0$, and $\bar{\phi}(g) = \bar{\phi}_3 \equiv 1 + p^2(1 + g)$ if $-1 < g$. Together with the self-consistency condition this leads to the following dependence of the order parameter $\bar{\phi}$ on the control parameter μ :

$$\bar{\phi}(\mu) = \begin{cases} \frac{\mu}{\alpha + q^{-2}}, & \mu < 0, \\ \frac{\mu}{\alpha - 1}, & 0 \leq \frac{\mu}{\alpha - 1} \leq 1, \\ \frac{\mu + 1 + p^{-2}}{\alpha + p^{-2}}, & \alpha - 1 < \mu. \end{cases} \quad (6)$$

The $\bar{\phi} - \mu$ characteristic of the uniform states is shown in Figure 1. It is easy to show that the uniform states corresponding to $\bar{\phi}_{1,3}$ are linearly stable, and that corresponding to $\bar{\phi}_2$ is unstable. Obviously, bistability of uniform states occurs only for $\alpha < 1$.

Due to the piecewise linearity of $f(\phi)$, the stationary KAP solutions can be constructed by matching hyperbolic and trigonometric functions. For the sake

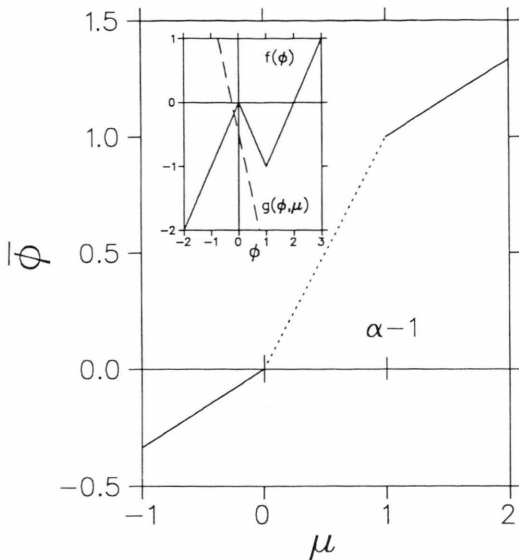


Fig. 1. Uniform solution $\bar{\phi}(\mu)$ obtained from $f = g$ (inset); $\alpha > 1$. The unstable part is indicated by the dotted line.

of brevity, we restrict ourselves to the case $\phi(x) \rightarrow \tilde{\phi}_1$ for large $|x|$:

$$\phi(x) = \begin{cases} \tilde{\phi}_1 + \hat{\phi}_1 \cosh\left(\frac{x - \frac{L}{2}}{q}\right), & x_a < |x| \leq \frac{L}{2}, \\ \tilde{\phi}_2 + \hat{\phi}_2 \cos(x + \varphi), & x_b \leq |x| \leq x_a, \\ \tilde{\phi}_3 - \hat{\phi}_3 \cosh\left(\frac{x}{p}\right), & 0 \leq |x| < x_b, \end{cases} \quad (7)$$

where the unknown variables $\hat{\phi}_{1,2,3}$, $x_{a,b}$ and φ are determined by the conditions of continuity and differentiability of $\phi(x)$ at $x_{a,b}$. The solution (7) exists only for $0 > g > g_{\text{eq}}$, where

$$g_{\text{eq}} = -1 / \left(1 + \sqrt{\frac{1+q^2}{1+p^2}} \right) \quad (8)$$

is associated with an equal-area rule [12] and characterizes an (anti-) kink connecting states with equal energy density. One can show that for $0 > g > g_1$, where $g_1 = -1/(1 + \sqrt{1+q^2})$, the KAP has for decreasing g a growing amplitude $\phi(0) \equiv \tilde{\phi}_2 + \hat{\phi}_2$ with $\hat{\phi}_2 = -g\sqrt{1+q^2}$, and fixed size, $x_a = \pi - \arctan(q)$, and $x_b \equiv 0$. On the other hand, if $g < g_1$ the size increases and diverges at $g \rightarrow g_{\text{eq}}$, where the amplitude saturates, i.e. $\phi(0) \rightarrow \tilde{\phi}_3$. In the latter case where $\phi(0) > 1$ it is convenient to parameterize the solution by x_b . One finds

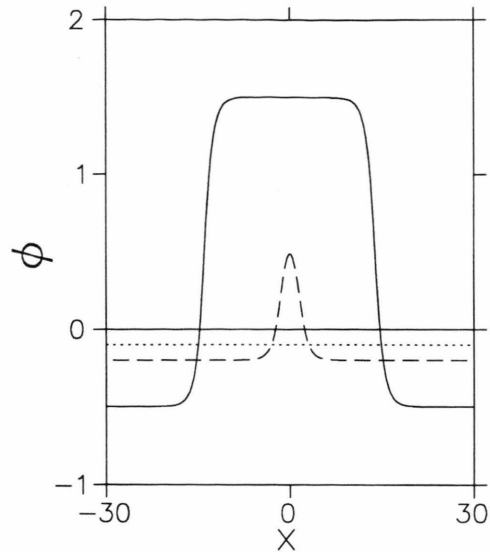


Fig. 2. Kink-antikink pairs for $g = -0.2$ (dashed), $g = g_{\text{eq}} + 10^{-12}$ (solid), and uniform state $\tilde{\phi}_1$ (dotted); $q = p = 1$.

$g = -(1 + \sqrt{(1+q^2)(1+p^2 \tanh^2(x_b/p))})^{-1})^{-1}$, $x_a = x_b + \pi - \arctan(q) - \arctan(p \tanh x_b/p)$, and $\hat{\phi}_3 = p^2(1+g)\sqrt{1 - \tanh^2(x_b/p)}$. The uniform state $\tilde{\phi}_1$ and the KAP for $g < g_1$ and $g > g_1$ are plotted in Fig. 2 as functions of x . The order parameter can be expressed in the form

$$\bar{\phi}(g) = \tilde{\phi}_1 + \frac{2}{L} \left((\tilde{\phi}_2 - \tilde{\phi}_1)(x_a + q) + (\tilde{\phi}_3 - \tilde{\phi}_2)(x_b - p \tanh(\frac{x_b}{p})) \right). \quad (9)$$

For $0 > g > g_1$ this gives $\bar{\phi}(g) = g(q^2 - 2(1+q^2)(x_a + q)/L) \approx q^2 g$, whereas in the limit of a strongly separated KAP, $g(\bar{\phi}, \mu) \cong g_{\text{eq}}$ implies

$$\bar{\phi} \cong \tilde{\phi}_1(g) + \Delta\phi(g) \frac{2x_b}{L}, \quad (10)$$

where $\Delta\phi \equiv \tilde{\phi}_3 - \tilde{\phi}_1 = \sqrt{(1+q^2)(1+p^2)}$ and $x_b \cong x_a$ is used.

From the self-consistency condition $\bar{\phi}$ and $x_{a,b}$ are obtained as functions of the control parameter μ . Standard stability analysis further shows that the stability of a KAP is equivalent to $(d\bar{\phi}/dg)\partial_{\bar{\phi}}g \geq 1$. Obviously, a negative slope $d\bar{\phi}/dg$ of the $\bar{\phi}$ - g characteristic is a necessary condition for stability of the localized state. The results are plotted in Figure 3. At $\mu = 0$ the unstable branch of a narrow KAP bifurcates subcritically

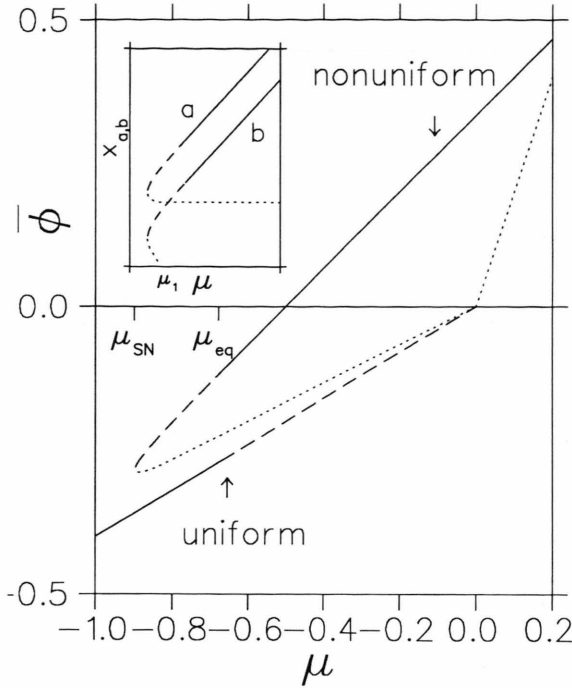


Fig. 3. $\bar{\phi} - \mu$ characteristic. The inset shows qualitatively $x_{a,b}(\mu)$. Stable, metastable, and unstable parts are indicated by solid, dashed, and dotted curves, respectively; $p = q = 1$.

from the uniform state. At the saddle-node bifurcation $\mu_{SN} \cong (1 + \alpha q^2)g_{eq} + \Delta\phi 2x_{SN}/L$ the unstable KAP merges with the stable KAP having a size

$$2x_{SN} \cong p \ln \left(\frac{4p(1 + g_{eq})^2}{\eta (\Delta\phi)^2} \right), \quad (11)$$

where $\eta = 2\alpha(1 + \alpha q^2)^{-1}L^{-1}$ can be understood as a measure for the strength of the nonlocal coupling of the domain walls.

The difference between the energies of a localized and the uniform state $\bar{\phi}_1$ is

$$\begin{aligned} \Delta E &= E[\phi] - E[\bar{\phi}_1] \\ &= -\frac{1}{2}\eta L^2(\bar{\phi} - q^2 g)^2 + \|\partial_x \phi\|^2, \end{aligned} \quad (12)$$

where g has to be taken at the KAP and where $\|\partial_x \phi\|^2$ is defined by

$$\begin{aligned} \int_{-L/2}^{L/2} dx (\partial_x \phi)^2 &= (1 + q^2)(x_a + q)g^2 \\ &\quad - (1 + p^2)(x_b - p \tanh(\frac{x_b}{p}))(1 + g)^2. \end{aligned} \quad (13)$$

We remark that in the local case (i.e. $\alpha = 0$) one finds the well-known result $\Delta E = \|\partial_x \phi\|^2$ [3] being constant in the limit of a well separated KAP, where $g = g_{eq}$.

The value μ_{eq} associated with equal energies of the stable KAP and the uniform state $\bar{\phi}_1$ (i.e. $\Delta E(\mu_{eq}) = 0$) turns out to be $\mu_{eq} \cong (1 + \alpha q^2)(g_{eq} + \|\partial_x \phi\|\sqrt{\eta})$, and the distance $2x_{eq}$ between kink and antikink is given by

$$x_{eq} \cong \frac{\|\partial_x \phi\|}{\Delta\phi} \sqrt{\eta^{-1}}. \quad (14)$$

Note that, whereas the critical size at the saddle-node bifurcation depends logarithmically on the sample length, i.e. $x_{SN} \propto \ln L$, it holds now $x_{eq} \propto \sqrt{L}$. In Fig. 3 one can see the $\bar{\phi} - \mu$ characteristics of the uniform state and the KAP, where the parts corresponding to linearly unstable and metastable states are indicated by dotted and dashed lines, respectively.

4. Nucleation

In this section, we assume that εF in (1) represents white noise of strength $2/\beta$ [3, 13, 14]. Then, in the region $\mu_{eq} < \mu < 0$ where $\bar{\phi}_1$ is metastable, a KAP can nucleate from this state via a fluctuation of an unstable KAP (the critical nucleus) in analogy to first-order phase transitions in equilibrium systems. Since the nucleation properties of this model have already been investigated in [13] and are similar to the local case studied in [14], we will restrict ourself to a brief review of the results concerning the strongly supersaturated case $g_1 < g < 0$. In the framework of a multi-dimensional Kramers theory one finds that the nucleation rate of noninteracting KAP's in the bulk is given by

$$r = L(1 + \mathcal{O}(\eta)) \chi(q) \frac{\lambda_s}{2\pi} \sqrt{\beta \Delta E} \exp(-\beta \Delta E), \quad (15)$$

where the growth rate λ_s of the breathing mode of the critical nucleus corresponds to the solution of $\sqrt{1 - \lambda} \sin(x_a) = \cos(\sqrt{1 - \lambda} x_a)$, and where $\chi(q) = \sqrt{q/(\pi(1 + q^2)(x_a + q))} \exp(x_a/q)$. Obviously, the form of (15) is in accordance with the well-known results of [3]. Therefore, one concludes

that the main effect of the nonlocality enters via the activation energy

$$\Delta E = \frac{(1+q^2)(x_a+q)}{(1+\alpha q^2)^2} \mu^2, \quad (16)$$

which is decreased for increased nonlocal coupling α and fixed control parameter μ , implying an increase of the nucleation rate. We expect a similar effect for the case of heterogeneous nucleation of KAP's at grain boundaries or at impurities [14].

5. Dynamics

In the presence of weak deterministic external forces εF , the dynamics of the stable KAP can be studied in the framework of a collective-coordinate ansatz, which is based on the existence of slow modes. These modes correspond to translations of the kink and the antikink, have vanishing or small restoring forces and give thus a large response to even small forces which break translational symmetry.

Let $\phi(x - x_0; \bar{x})$ denote the unperturbed solution which describes a KAP of size $2\bar{x}$ and centered at x_0 . The projection of (1) onto $\partial_{x_0}\phi$ and $\partial_{\bar{x}}\phi$ yields

$$\dot{x}_0 = -\frac{\varepsilon}{\|\partial_x \phi\|^2} \int dx \partial_x \phi(x - x_0; \bar{x}) \cdot F[\phi(x - x_0; \bar{x}), x], \quad (17)$$

$$\dot{\bar{x}} = M(\bar{x}) + \frac{\varepsilon}{\|\partial_x \phi\|^2} \int dx \partial_{\bar{x}} \phi(x - x_0; \bar{x}) \cdot F[\phi(x - x_0; \bar{x}), x]. \quad (18)$$

One finds in leading order of $g - g_{\text{eq}}$ and $\exp(-2\bar{x}/p)$

$$M(\bar{x}) = -\frac{2}{\|\partial_x \phi\|^2} (V(\tilde{\phi}_3, g) - V(\tilde{\phi}_1, g)) - \frac{4p^2(1+g)^2}{\|\partial_x \phi\|^2} \exp(-2\bar{x}/p), \quad (19)$$

where $V(\tilde{\phi}_3, g) - V(\tilde{\phi}_1, g) \cong \Delta\phi(g - g_{\text{eq}})$ is the difference of the local energy densities of the different domain states $\tilde{\phi}_3$ and $\tilde{\phi}_1$. The self-consistency condition reads for large L

$$g = \frac{\mu - \alpha(1+p^2)2\bar{x}/L}{1 + \alpha q^2}. \quad (20)$$

We will assume a very stiff KAP, which means that ε is small such that time scales associated with the translation mode and the breathing mode of the KAP separate. This means that the center of mass of the rigid KAP obeys approximately (17) at *fixed* size.

As a first approximation, the size $2\bar{x}$ of the KAP follows instantaneously according to (18) and is thus slaved by the slow motion of the KAP. From (18), (19), and (20) one obtains the relaxation constant λ_f of the KAP size by linearization ($\bar{x} \rightarrow \bar{x} + \delta\bar{x} \exp(\lambda_f t)$)

$$\lambda_f = \frac{2}{\|\partial_x \phi\|^2} \left(-(\Delta\phi)^2 \eta + 4p(1 + g_{\text{eq}})^2 \exp(-\frac{2\bar{x}}{p}) \right). \quad (21)$$

The first term in the large bracket can be associated with the nonlocal inhibition which stabilizes the KAP. The second term, which describes the kink-antikink interaction, can be neglected if $\bar{x} \gg x_{SN}$. We proceed with an example.

6. Pinning and Mobility

We consider a weak force with

$$F[\phi, x, t] = -v \partial_x \phi + \sum_j \delta(x - r_j), \quad (22)$$

which describes an external field v acting on the KAP and which contains the influence of a diluted density ρ ($\ll 1/d$) of $N = \rho L$ localized pointlike and attracting impurities located at r_j . ‘Diluted’ means that the probability of two walls being at the same time near impurities can be neglected. Equation (17) can be written in the form

$$\dot{x}_0 = v + K(x_0) \equiv v + \frac{1}{\|\partial_x \phi\|^2} \sum_j \partial_x \phi(x_0 - r_j), \quad (23)$$

where the dot denotes differentiation with respect to the rescaled time $t \rightarrow \varepsilon^{-1}t$, corresponding to a slow motion.

We are mainly interested in the average velocity $v_{\text{eff}} \equiv mv$ and the average elongation $2\Delta\bar{x}$ of the KAP. In order to get a finite mobility m , the modulus of v has to be larger than the depinning field $v_c = \phi_2/\|\partial_x \phi\|^2$ such that the KAP can be pulled away from a pinning center. For distances X very large compared to the average distance of the impurities and

for times T such that $X = v_{\text{eff}}T$ holds, the mobility obeys

$$m^{-1} \equiv \frac{v}{v_{\text{eff}}} = \frac{1}{X} \int_0^X \frac{dx}{1 + K(x)/v}. \quad (24)$$

This expression can be evaluated by expanding the geometric series and integrating while neglecting the events where both domain walls cross impurities at the same time:

$$\begin{aligned} m^{-1} &= 1 + \frac{2N}{L} \sum_{n=1}^{\infty} (v \|\partial_x \phi\|^2)^{-2n} \\ &\quad \cdot \int_0^{L/2} dx (\partial_x \phi(x))^{2n} \\ &= 1 + \rho (b_m(v, q) + b_m(v, p)), \end{aligned} \quad (25)$$

where

$$\begin{aligned} b_m(v, y) &= \frac{\pi - 2 \arctan zy}{z} - (\pi - 2 \arctan y) \\ &\quad + y \ln\left(\frac{1 + y^2}{1 + (zy)^2}\right), \end{aligned} \quad (26)$$

and where $z := \sqrt{1 - (v_c/v)^2}$.

We calculate similarly the average change $\Delta \bar{x} = \bar{x} - \bar{x}_{\varepsilon=0}$ to first order of ε . On the one hand, if $v > v_c$, the time average of $\Delta \bar{x}$ becomes

$$\begin{aligned} \langle \Delta \bar{x} \rangle &= \frac{m}{X} \int_0^X \frac{\Delta \bar{x}(x) dx}{1 + K(x)/v} \\ &= -\rho \frac{\varepsilon |v|}{\lambda_f} \left(b_{\bar{x}}(v, q) + b_{\bar{x}}(v, p) \right), \end{aligned} \quad (27)$$

where

$$\begin{aligned} b_{\bar{x}}(v, y) &= 2m \left(y \operatorname{arctanh}\left(\frac{y v_c/|v|}{\sqrt{1 + y^2}}\right) \right. \\ &\quad \left. + z^{-1} \arctan\left(\frac{v_c/|v|}{z \sqrt{1 + y^2}}\right) \right) \end{aligned} \quad (28)$$

and where $\Delta \bar{x}(x)$ has been approximated by adiabatic elimination in (18). On the other hand, one finds for the elongation of the separation of the pinned KAP (i.e. $v < v_c$) the result $2\Delta \bar{x} = -2\varepsilon|v|/\lambda_f$, which is roughly the ratio of the strength of the external force and the stiffness of the KAP.

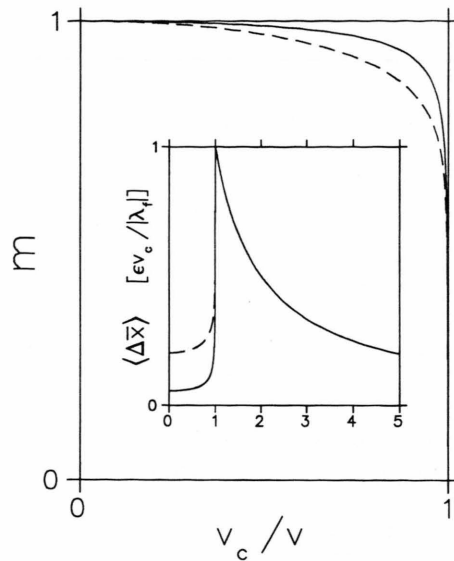


Fig. 4. Mobility m of the KAP and average change of \bar{x} (inset) as a function of v_c/v in the presence of impurities and an external driving force. Note that $v_c/v > 1$ belongs to the pinned KAP; $p = q = 1$ (solid), $p = q = 2$ (dashed).

The mobility and the elongation are shown in Fig. 4 as a functions of the inverse driving force $|v/v_c|$. One finds the following behavior. As one expects, $m \rightarrow 1$ if $v/v_c \rightarrow \infty$, i.e. a very quickly moving KAP does not feel the impurities. Furthermore, for $v \searrow v_c$ it holds $v_{\text{eff}} \approx \sqrt{v_c/2} \sqrt{v - v_c} L / \pi N$; since the KAP stays for a long time close to the impurity if the field v has values only slightly above the depinning field, $m \rightarrow 0$ for $|v| \searrow v_c$.

The maximal change of the size of the KAP appears at the depinning field, $|v/v_c| \rightarrow 1$, and is given by $2\langle \Delta \bar{x} \rangle \rightarrow -2\varepsilon v_c / \lambda_f$, which is in accordance with the case where the KAP is pinned. In the limit of large fields, $|v/v_c| \rightarrow \infty$, one finds that $\langle \Delta \bar{x} \rangle \rightarrow \varepsilon v_c 2\rho \sqrt{1 + p^2} / g \lambda_f$. For a fast moving KAP the relative influence of the impurities decreases and hence $\langle \Delta \bar{x} \rangle$ decreases and goes to a finite value.

7. Summary

In this paper we investigated the statics, the nucleation and the dynamics of stable kink-antikink pairs in a simple reaction-diffusion model. Stable KAP's can exist in the presence of strongly nonlocal inhibition and bifurcate at a saddle-node bifurcation with a characteristic size $\propto \ln L$. They turn out to become globally stable at a characteristic size $\propto \sqrt{L}$.

In the region, where the uniform state is metastable, the nucleation rate of a KAP differs from the local case mainly by the decrease of the activation energy. Furthermore, we studied the dynamics of the KAP under the influence of weak external forces by using the slowness of translation and breathing modes. In particular, we discussed as an example the pinning and mobility properties of a driven KAP in a sample containing impurities.

Acknowledgements

The author is very grateful to H. Thomas and F. J. Elmer for many stimulating discussions. The content of this paper was part of the Ph. D. thesis of the author at the University of Basel and was supported by the Swiss National Science Foundation. It was a great pleasure to present these results at the 5th Annual Meeting of the ENGADYN Workshop in Grenoble.

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