Nucleation of Weakly Driven Kinks

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We study nucleation of kink-antikink pairs under weak nonequilibrium conditions and in the strong friction limit. We introduce an effective critical nucleus of size s_0, which is small compared to the inverse kink density but large compared to a kink size. We evaluate independently the nucleation rate and the kink lifetime from a multidimensional Kramers theory and by studying kink-antikink annihilation processes. We find a kink density which is independent of s_0 and of the driving force in this regime. The result is in accordance with the equilibrium kink density obtained from statistical mechanics.

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The nucleation and dynamics of solitary structures in spatially one-dimensional and multistable systems are of great interest in theoretical [1–9], experimental [10], and computational [11,12] physics. In such systems the fundamental kinetic processes are a nucleation of kink-antikink pairs, their subsequent propagation, and their eventual annihilation. It is the purpose of this Letter to discuss these kinetic coefficients near equilibrium, where the external driving force F is very small. This regime is difficult to analyze, since a naive extension of the well-established nucleation theory for large F yields a critical nucleus with a size that diverges at equilibrium. At small temperatures, the density of kinks and antikinks is finite and sets an upper length scale over which nucleation and annihilation processes have to occur. In the framework of equilibrium statistical mechanics, moreover, kinks and antikinks are regarded as free particles. For reasons of consistency, it is thus necessary to develop a picture of the nucleation and annihilation processes which permits essentially free diffusive motion during the lifetime of a kink.

A theory of kink dynamics in multistable systems was outlined already in the mid-fifties in connection with dislocation theory by Seeger [1] and Lothe and Hirth [2]. Much work has been focused on the overdamped sine-Gordon chain subject to a driving force and to thermal noise. A quantitative theory which permitted the evaluation of the average speed and the discussion of fluctuations away from this average behavior was developed by Büttiker and Landauer [6], where the nucleation rate and the annihilation rate were evaluated for driving forces so large that a kink-antikink pair which has nucleated is driven apart. In this regime, the kink motion during the lifetime of the kink is purely deterministic, and a kink annihilates with probability 1 with an antikink being generated by another nucleation event. However, this is no longer true for weak driving forces. Here, diffusion of kinks and antikinks becomes important. The case of moderate and weak forces was treated by Hänggi, Marchesoni, and Sodano [8]. Although one expects in the equilibrium limit a nucleation rate with an activation energy $2E_k$ of the nucleus, which is *twice* the kink energy, an activation energy of $3E_k$ has been predicted by Ref. [8], and subsequently by Refs. [9,12]. However, we will show that careful definitions of nucleation and recombination processes yield a different result, namely, the expected dependence on the activation energy $2E_k$.

The dynamics of kinks and antikinks in space-time is schematically illustrated in Fig. 1. In the driven case, part (a), a kink and an antikink are driven apart after a nucleation process (empty triangles) and annihilate eventually with an antikink and a kink originating from a different nucleation process (rectangles). Obviously, this picture cannot be applied in the equilibrium case shown in part (b). Here the diffusive motion of the free kinks gives them a *strongly enhanced probability of returning to its nucleation partner*. The history of kinks which annihilate with their original antikink is represented by closed loops (bubbles) in Fig. 1(b). Only a negligible small fraction of extended trajectories exists. The works [8,9,12] which arrive at a nucleation rate with activation energy $3E_k$

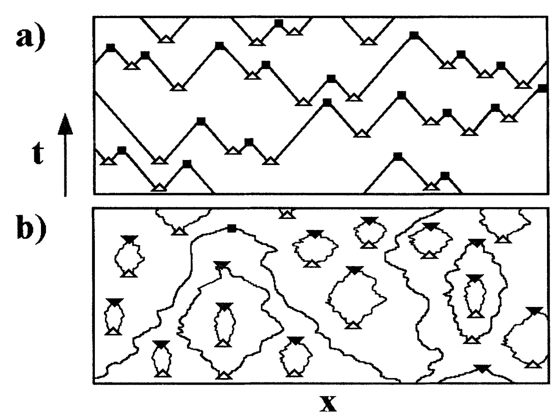

FIG. 1. Space-time plot of the dynamics of kinks and antikinks. In the driven case [part (a)] the motion is mainly a drift; kink and antikink of a nucleation process (empty triangles) recombine with different antikinks and kinks (full rectangles). At equilibrium [part (b)], the motion is diffusive; nucleation and annihilation of the same pair (full triangles) dominates.

consider only the open trajectories and neglect the closed ones. As a consequence, these works predict a kink lifetime proportional to $\exp(2E_k/kT)$, whereas the theory presented below leads to a kink lifetime proportional to $\exp(E_k/kT)$. Neglecting the closed trajectories is inconsistent with the experimental definition of free kinks. All kinks represented in this figure contribute to the kink density. Let us present now a natural way of treating the equilibrium case.

Effective nucleus.—In order to overcome the problem of the large critical nucleus, we introduce an *effective critical nucleus* with a separation s_0 of the kink and the antikink, which is much larger than a kink width but much smaller than an average equilibrium separation of kinks. This is a key step in our work. Below we show that the equilibrium kink lifetime τ_{eq} depends on s_0 and is given by

$$\tau_{\mathrm{eq}} = \frac{s_0}{2Dn}, \tag{1}$$

where n and D are the kink density and the diffusion constant, respectively. Note that this is where we differ from previous treatments, where $\tau \approx 1/n^2$ is assumed [8]. Since the nucleation rate j is proportional to n/τ, we will find $j \propto n^2 \propto \exp(-2E_k/kT)$ instead of $j \propto n^3 \propto \exp(-3E_k/kT)$.

The effective critical nucleus is associated with a closed trajectory of minimal (spatial) size s_0 in Fig. 1(b). This size is thus a (spatial) cutoff length of the closed trajectories. The energy of an undriven pair as a function of the separation coordinate s is shown by the full curve in Fig. 2. The well A corresponds to a given uniform state. For the sine-Gordon system it is important to distinguish between the rates j_+ and j_- associated with a nucleation of a kink-antikink pair (B_+) and an antikink-kink pair (B_-). An energy slightly less than $2E_k$ is needed to form a pair. For $s \approx s_0$ the energy still increases with s but only exponentially weakly due to the typical long-distance interaction of a kink and an antikink [7]. In this regime

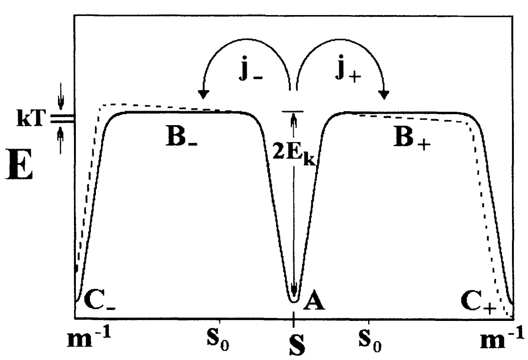

FIG. 2. Qualitative dependence of the energy on the kink-antikink separation s. $j_\pm$ denote nucleation rates of free kinks ($B_\pm$) out of the valley A. Recombination processes correspond to the fall back into A, or into the wells $C_\pm$ which illustrate antikinks created by other nucleation events ($\pm$ indicates pairs associated with droplets corresponding to different Peierls valleys).

they can already be regarded as free diffusing particles. In contrast to the strongly driven case, a free kink has the possibility to annihilate with the antikink with which it was generated. In Fig. 2 this corresponds to a return to A. On the other hand, the kink will leave the antikink with a certain probability and eventually annihilate with an antikink that was generated independently. This process is illustrated in Fig. 2 by falling from $B_\pm$ into the well $C_\pm$. The mean separation of A and $C_\pm$ is given by the inverse antikink density m^{-1}. Below, periodic boundary conditions will be assumed which allow one to set finally m equal to the stationary kink density n.

It is important to realize that the kinks in the flat portion of this energy diagram are those that are counted if one evaluates the kink density within equilibrium statistical mechanics. Thus the choice of the size s_0 of the critical nucleus is to some extent arbitrary. This choice affects kinetic quantities like the kink nucleation rate and the kink lifetime. However, as we will show, stationary quantities such as the stationary kink density n are independent of this choice as long as s_0 is small enough. We emphasize again the internal consistency of our approach: Below we evaluate the kink nucleation rate and the kink lifetime *independently* and use these results to find the kink density n.

Before presenting our calculation, let us briefly discuss the energy diagram if a small driving force is applied. This corresponds to the dashed curve in Fig. 2. The rates j_+ and j_- can now be associated with nucleation processes in the direction of the field and against the direction of the field, respectively. Different regimes can be distinguished depending on the strength of the applied force F. In the *diffusive regime* the applied driving force is so small that the energy $2\pi F n^{-1}$ gained by a kink from the driving force over the interkink distance is small compared to the thermal energy kT. This situation is essentially the same as at equilibrium. In the *weakly driven regime*, where the applied force exceeds

$$F_{\mathrm{cr},1} = nkT/2\pi, \tag{2}$$

the drift induced by the external field becomes important. However, in this weakly driven regime kinks still have a substantial probability to annihilate with the partner antikink. To suppress the annihilation with the partner antikink we need a driving force which exceeds

$$F_{\mathrm{cr},2} = kT/2\pi s_0. \tag{3}$$

For driving forces $F \gg F_{\mathrm{cr},2}$ we enter the *strongly driven regime* where the applied force is sufficiently strong to separate a pair with large probability [Fig. 1(a)]. This strongly driven regime was the main subject of Ref. [6]. Here we emphasize the diffusive regime and the weakly driven case where $F \leq F_{\mathrm{cr},2}$ [Fig. 1(b)].

Model.—The model which we will consider is the overdamped sine-Gordon equation [3]

$$\gamma \partial_t \theta = -V_0 \sin\theta + F + \kappa \partial_x^2 \theta + \zeta, \tag{4}$$

which describes the overdamped dynamics of the order-parameter field $\theta(x,t)$ in a periodic potential of amplitude V_0, with a damping constant γ, a diffusion constant κ, and subject to the driving force F. We can assume $F \geq 0$ without the loss of generality. As mentioned above we assume periodic boundary conditions $\theta(L + x, t) = \theta(x, t)$, where L is the sample length which exceeds every other relevant length scale of the problem (except probably the diverging size of the exact nucleus). The small stochastic force ζ with zero mean $\langle \zeta \rangle = 0$ has a strength $\langle \zeta(x,t)\zeta(\tilde{x},\tilde{t})\rangle = 2\gamma kT\delta(x - \tilde{x})\delta(t - \tilde{t})$, where kT is the thermal energy, and the occurrence of γ reflects the fluctuation-dissipation theorem. Let us recall some properties [6] of Eq. (4). Multistability occurs for values $F < V_0$. The uniform, stationary, and linearly stable states are given by $\theta_{s,l} = 2l\pi + \arcsin(F/V_0)$ (Peierls valleys) with integer l. There exists an energy functional $E[\theta]$ such that Eq. (4) can be rewritten in the form $\gamma \partial_t \theta = -\delta E[\theta]/\delta\theta$. Under equilibrium conditions (i.e., $F = 0$) all the $\theta_{s,l}$ have the same energy. In the presence of a nonvanishing force ($0 < F < V_0$) the stationary solutions $\theta_{s,l}$ constitute a set of metastable states. Two adjacent Peierls valleys are separated in function space by a saddle which corresponds to a kink-antikink pair. A kink $\theta_k(x - x_0)$ centered at x_0 connects a Peierls valley $\theta_{s,l}$ with its neighbor $\theta_{s,l+1}$. An antikink is reversely defined by $\theta_a = \theta_k(-x + x_0)$. Hence a kink-antikink pair at location x_0 and with a (not too small) separation s can be written approximately as $\theta_N(x) = \theta_k(x - x_0 + s/2) + \theta_k(-x + x_0 + s/2) - 2\pi(l + 1)$. The *exact* critical nucleus being an exact saddle point of the energy functional corresponds to a pair with a separation $\xi = \xi_0 \ln(V_0/F)$, where $\xi_0 = \sqrt{\kappa/V_0}$ is the kink size. In the weakly driven case, F can be arbitrarily small such that the separation ξ is larger than the inverse kink density n^{-1} or even larger than the system length L. In this case, the mathematically exact critical nucleus has no physical meaning.

Balance equation.—The stationary kink density n can be obtained from a balance equation. Imagine that the average kink lifetime $\tau_\pm = \tau(\pm F, m)$ for given F and the fixed antikink density m is known. Here τ_+ and τ_- refer to kink-antikink pairs and to antikink-kink pairs, respectively. The stationarity condition requires that the nucleation rates $j_\pm$ of the kinks be equal to their recombination rates $n_\pm/\tau_\pm$. Here n_+ and n_- denote densities of kink-antikink pairs and antikink-kink pairs, respectively. The symmetry of the sine-Gordon equation implies $= j_+(-F) = j_-(F)$. The total kink density $n = n_+ + n_-$ is then given by the implicit Equation

$$j_+ \, \tau_+ \; + \; j_- \, \tau_- = n \, . \tag{5}$$

One concludes from this result that the stationary kink density is an even function of F.

Kink lifetime.—The kink lifetimes $\tau_\pm$ for fixed antikink density m can be calculated with the help of a Langevin equation for the kink separation s. This Langevin equation follows from a projection of the Eq. (4) onto the quasi-Goldstone mode $\delta\theta_N/\delta s = \theta_k'(x - x_0 + s/2)/2 + \theta_k'(-x + x_0 + s/2)/2$ associated with an infinitesimal variation of s. Note that there is also an orthogonal Goldstone mode $\delta\theta_N/\delta x_0 = \theta_k'(-x + x_0 + s/2) - \theta_k'(x - x_0 + s/2)$ associated with an infinitesimal displacement δx_0 of the pair. The Fokker-Planck equation, which is equivalent to the Langevin equation, reads in the stationary case $\partial_s(\pm\tilde{F}P - \tilde{D}\partial_s P) = 0$, with an effective force $\tilde{F} = 2\mu F$ and diffusion constant $\tilde{D} = 2\mu kT/2\pi$. Here, $\mu = 2\pi\kappa/\gamma E_k$ is the kink mobility. Note that the values of $\tilde{F}$ and $\tilde{D}$ for the relative coordinate s are twice as large as for a single kink. The stationary Fokker-Planck equation must be solved with a source at $s = s_0$ and with sinks at $s = 0$ and $s = m^{-1}$ (see Fig. 2). The source describes the nucleation of a pair, and the sinks model kink-antikink annihilation. The stationary Fokker-Planck equation is of the form $\partial_s J = 0$ and can, therefore, be integrated. This leads to a constant current density J. However, the source implies a discontinuity of the current density of strength $j_\pm$ at s_0. The absorbing boundary conditions demand $P(0) = P(m^{-1}) = 0$. The lifetimes $\tau_\pm$ are defined by the ratio of the total probability $\int ds\, P$ and the injected current $j_\pm$. We find

$$\tau_\pm = \pm\frac{s_0}{\tilde{F}}\left(\frac{1}{s_0 n}\,\frac{1 - \exp(\mp\tilde{F}s_0/\tilde{D})}{1 - \exp(\mp\tilde{F}/n\tilde{D})} - 1\right), \tag{6}$$

where m has been replaced everywhere by n. This result indicates the existence of the above mentioned three different regimes of the force. Let us first give a remark on the strongly driven case, where F/V_0 cannot be neglected in the nucleation rate [6,8]. Then the nucleation rate j_- is exponentially suppressed and the total nucleation rate j equals j_+. Obviously, $n_0 = n_+$ holds, and from Eq. (6) $\tau(n) = 1/\tilde{F}n$ follows. The rate obtained from Eq. (5) becomes finally $j = 2un^2$, with the kink velocity $u = \tilde{F}/2$. This result is in accordance with the nondiffusive limit discussed in Refs. [5,6].

On the other hand, the equilibrium-kink lifetime given by Eq. (1) follows from Eq. (6) by setting $F = 0$.

Nucleation rate.—Let us now derive the nucleation rates $j_\pm$. Within multidimensional Kramers theory [13], the rate is calculated by solving a stationary Fokker-Planck equation in the function space $\{\theta(x)\}$. Usually, one prescribes a normalized and thermalized populations in the metastable well, imposes an absorbing boundary condition beyond the saddle, and determines the stationary flux $j_\pm$ across the saddle. Here, we have to proceed differently, since we deal with nucleation into a region which is exponentially flat (Fig. 2).

The above emphasized exponential flatness of the saddle is taken into account in the following way. Firstly, since the kink is considered to be free for $s > s_0$, we must impose the absorbing boundary at $s = s_0$. Secondly, due to the existence of the quasi-Goldstone mode, the integration across the saddle in function space cannot be treated anymore by a Gaussian approximation as in the usual case where the saddle has a finite curvature. It rather has to be treated similar to the translational Goldstone mode and leads to a term proportional to s_0. By proceeding as in Ref. [6] but taking into consideration the differences just mentioned, the rate per length can be expressed by

$$j_{\pm} = \frac{1}{L} \frac{\tilde{Z}_N}{\tilde{Z}_s} \frac{\int_0^{\eta_1(L)} d\eta_1}{\int_0^{\eta_0(s_0)} d\eta_0} \exp(-E_N/kT). \quad (7)$$

Here, terms of order $2\pi F s_0/kT$ and of order F/V_0 are neglected. Hence the activation energy is simply given by $E_N = 2E_k$, where $E_k = 8\sqrt{\kappa V_0}$ is the equilibrium-kink energy [6]. The ratio

$$\frac{\tilde{Z}_N}{\tilde{Z}_s} = \frac{1}{2\pi}\sqrt{\lambda_0^s \lambda_1^s \prod_{n=2}^{\infty} \frac{\lambda_n^s}{\lambda_n^N}} \quad (8)$$

contains the stability eigenvalues $\lambda_n^{s,N}$ of the metastable state (index s) and the critical nucleus (index N) with respect to perturbations $\propto \exp(\lambda t)$. As usual, the (quasi-) zero modes are excluded in the products. For a well-separated pair, Eq. (8) is the normalized partition function of a kink-antikink pair without self-interaction and is given by $\tilde{Z}_N/\tilde{Z}_s = 4\Gamma/2\pi$, where $\Gamma = V_0/\gamma$ and where terms of the order F/V_0 are neglected [6]. The variables η_0 and η_1 are the orthonormal-mode coordinates which belong to the kink-separation mode and the translational mode. It holds [6]

$$d\eta_0^2 = ds^2 \int (\delta\theta_N/\delta s)^2 dx\,,$$
$$d\eta_1^2 = dx_0^2 \int (\delta\theta_N/\delta x_0)^2 dx\,. \quad (9)$$

Using the quasi-Goldstone and the Goldstone modes given above, one finds for the ratio of the integrals in Eq. (7) a value $2L/s_0$. The nucleation rate becomes finally

$$j_- = j_+ = \frac{4\Gamma}{\pi s_0} \exp(-2E_k/kT). \quad (10)$$

The stationary kink density n follows immediately from Eqs. (5), (6), and (10):

$$n = n_{\rm eq} = \sqrt{\frac{2V_0 E_k}{\pi\kappa kT}} \exp(-E_k/kT). \quad (11)$$

This is the equilibrium kink density $n_{\rm eq}$ found in Ref. [6] from equilibrium statistical mechanics. By deriving Eq. (11) we used that $\tau_+ + \tau_- = s_0/n\tilde{D} = 2\tau_{\rm eq}$ for $F \ll F_{{\rm cr},2}$, which is independent of $F/F_{{\rm cr},1}$. This follows from the specific symmetry of the sine-Gordon equation, and is different, for example, in a bistable system where only a single saddle exists for a given valley [4,11,12].

The stationary kink density (11) is independent of the specific value of s_0. The kinks to be counted at a fixed time t must be nucleated in a strip of width $\tau \propto s_0$ in Fig. 1(b). Since the nucleation rate per length is proportional to $1/s_0$, one finds a kink density independent of s_0. A variation of s_0 affects only the time scale but not stationary quantities.

Our result is valid for $1/n \gg s_0 \gg \xi_0$, with the kink width $\xi_0 = \sqrt{\kappa/V_0}$, and for $2\pi F s_0 \ll kT$. These conditions can only be satisfied if $F \ll kT/2\pi\xi_0$. Since Kramers theory is valid for $kT \ll E_N = 16\sqrt{\kappa V_0}$, one concludes that also $F \ll V_0$ is satisfied.

Our approach permits the investigation of the fluctuation spectra of kink and antikink densities [5] close to equilibrium over a much larger range of frequencies than was previously possible. Now, the density-density correlation spectra are expected to depend on s_0. A discussion of the fluctuation problem will be provided elsewhere.

In summary, we have developed a theory of kink nucleation near equilibrium by introducing an effective size s_0 of the critical nucleus. It turns out that the nucleation rate depends on the usual Arrhenius factor containing the activation energy $2E_k$ of the nucleus, and the equilibrium kink lifetime is proportional to $\exp(E_k/kT)$. Although our result has to be expected, it is new and in contrast to earlier theories. The kink density n is independent of both s_0 and of the force F as long as $2\pi F s_0 \ll kT$. This density is in accordance with the result obtained from equilibrium statistical mechanics.

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