Asymmetric Kinks: Stabilization by Entropic Forces

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Asymmetric kinks bridging two adjacent potential valleys of equal depth but different curvature are unstable against phonon modes. When coupled to a heat bath, a kink-bearing string tends to cross over into the shallower valley; kinks are thus predicted to drift in the appropriate direction with velocity proportional to the temperature, in close agreement with numerical simulation. When contrasted by a mechanical bias, these entropic forces give rise to a rich phenomenology that includes configurational phase transitions, double-kink dissociation, and noise-directed signal transmission.

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The Brownian motion of asymmetric solitons provides an analytically tractable example of how thermal fluctuations in extended systems may generate temperature dependent *entropic* forces, besides the customary *stochastic* forces responsible for diffusive processes.

Let us consider an elastic string at finite temperature, confined to a symmetric bistable potential subjected to an *external* tilt. The system overall is asymmetric; the minima of the tilted potential are separated by an energy gap $\Delta\epsilon$ but, as long as the tilt may be treated as a perturbation, their curvatures remain the same. On bridging the two parallel valleys, the string forms symmetric solitons (kinks and antikinks); solitons are unstable under translations (namely, undergo Brownian motion driven by a drift force proportional to $\Delta\epsilon$), but their shape is not deformed appreciably [1–3].

A different type of asymmetry manifests itself when the string potential is *internally* deformable [4], so that the energy gap $\Delta\epsilon$ may vanish, but the curvatures at the valley bottoms grow different. In this case the very profile of the string solitons is asymmetric and thermal fluctuations seem to push them sidewise, as noticed first in an earlier numerical study [5]. Effects related to this type of asymmetry have not been investigated any further even if they may affect dramatically the transport properties of string models of wide application in solid state physics (dislocations, magnetic flux lines in type-II superconductors), biophysics (neuron signal propagation, polymer chains) and statistical mechanics (domain walls in order-disorder transitions).

In this Letter, we address a fairly simple question. Look at the tilted bistable potential $V[\phi]$ in Fig. 1 with the left valley 1 lower but narrower than the right valley 2; suppose that the elastic string $\phi(x,t)$ rests across the potential barrier (centered at $\phi = \phi_0$) so as to form a kink ϕ_{12} as shown, i.e., $\phi_{12}(x \to -\infty) = \phi_1$ and $\phi_{12}(x \to +\infty) = \phi_2$; let the string be subjected to equilibrium thermal fluctuations with temperature T and strong viscous coupling (without loss of generality we can restrict our discussion to the overdamped regime): In which direction will the kink ϕ_{12} drift under the combined action of the external tilt and the internal potential asymmetry?

A simple energetic argument, certainly valid in the (0 + 1)D case of a single Brownian particle, suggests that ϕ_{12} ought to travel to the right as the string would sit preferably in the lower valley. We show here that the actual behavior of an asymmetric kink is more complicated and depends *critically* on the string temperature.

The string dynamics is modeled by the field equation

$$\phi_{tt} - c_0^2\phi_{xx} + \omega_0^2 V'[\phi] = F - \alpha\phi_t + \zeta(x,t), \quad (1)$$

where c_0 is the limiting propagation speed of a phonon pulse, ω_0^2 is the (maximum) potential barrier height, and F is a tunable external tilt, we introduce as an auxiliary control parameter for later use. The coupling to an *equilibrium* heat bath is characterized by the viscous damping constant α and the Gaussian noise $\zeta(x,t)$ with zero mean and autocorrelation function

$$\langle\zeta(x,t)\zeta(x',t')\rangle = 2\alpha kT\,\delta(x - x')\delta(t - t'). \quad (2)$$

The local minima $\phi_{1,2}$ of the bistable potential $\omega_0^2 V[\phi]$ are a distance $a \equiv \phi_2 - \phi_1$ apart, differ by the energy gap $\Delta\epsilon \equiv \omega_0^2(V[\phi_2] - V[\phi_1])$, and their curvatures $\omega_{1,2}^2 \equiv \omega_0^2 V''[\phi_{1,2}]$ control the asymmetry of the kink ϕ_{12} through the parameter $\Delta\omega \equiv \omega_1 - \omega_2$. For convenience we choose $\Delta\epsilon \geq 0$ and $\Delta\omega \geq 0$.

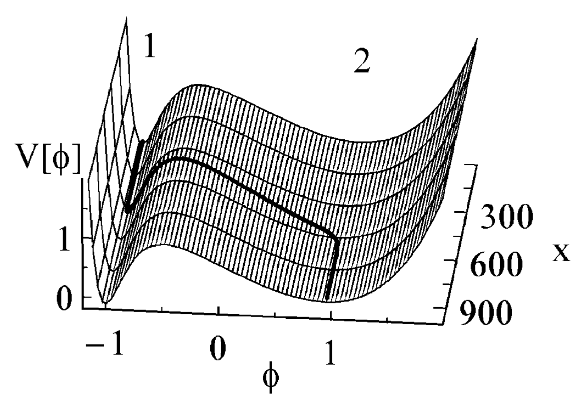

FIG. 1. Kink in a tilted asymmetric potential. Potential $V[\phi]$ and other string parameters are specified in Fig. 3.

Let us consider first the simpler case of an *unbiased* kink, that is a potential $V_0[\phi]$ with degenerate minima, say $V_0[\phi_{1,2}] = 0$, so that $\Delta\epsilon = 0$. The corresponding unperturbed kink $\phi_{12}(x,t)$ is a solution of Eq. (1) with $\alpha = T = F = 0$ [i.e., zero right-hand side (rhs)]; its implicit form [6]

$$x - ut = \left(1 - \frac{u^2}{c_0^2}\right)^{1/2} \frac{d}{\sqrt{2}} \int_{\phi_0}^{\phi_{12}(x-ut)} \frac{d\phi}{\sqrt{V_0[\phi]}} \qquad (3)$$

describes a relativistic quasiparticle with size $d \equiv c_0/\omega_0$, constant speed u with $|u| < c_0$, rest energy

$$E_0 = \omega_0 c_0 \int_{\phi_1}^{\phi_2} \sqrt{|2V_0[\phi]|}\, d\phi\,, \qquad (4)$$

and mass $M_0 = E_0/c_0^2$. The antikink $\phi_{21}(x,t)$ is defined through Eq. (3) upon reversing the sign of its rhs.

The stability analysis of an unbiased asymmetric kink [4] is illustrated in Figs. 2(a) and 2(b). In linear approximation small kink deformations are expandable on the basis of the orthogonal eigenfunctions $\chi(x,t) = \psi(x)e^{-i\omega t}$ with

$$-c_0^2\psi_{xx} + \tilde{V}_0(x)\psi = \omega^2\psi\,. \qquad (5)$$

This stability equation is easily mapped into a one-dimensional Schrödinger equation for the asymmetric well $\tilde{V}_0(x) \equiv \omega_0^2 V_0''[\phi_{12}^{(0)}]$, where $\phi_{12}^{(0)}$ denotes a static kink centered, say, at the origin [note that $\lim_{x\to\pm\infty}\tilde{V}_0(x) = \omega_{2,1}^2$, see Fig. 2(b)]. The Goldstone mode $\omega = 0$ governs the kink translation, while the phonon modes with $\omega_k^2 > \omega_2^2$ exert a net pressure on the kink ϕ_{12}. This property is apparent in the frequency range (ω_2, ω_1): phonons impinging on the kink from the right get reflected back, thus nudging it to the left.

As the unbiased kink ϕ_{12} is unstable under small oscillations, we expect that thermal fluctuations push it to the left, likewise [5]. In order to estimate the ensuing thermal force $F_{\rm th}$ acting upon the kink center of mass, we turn a *stopping* tilt F on, so that kinks ϕ_{12} and antikinks ϕ_{21} form a dilute gas in thermal equilibrium [i.e., zero net (anti)kink current]. In the transfer-matrix formalism [6–8] this corresponds to imposing the "tunnel-splitting" condition in the eigenvalue problem for the kink-antikink gas free-energy,

$$\hat{H}[\phi]\eta_n[\phi] = \epsilon_n \eta_n[\phi], \qquad (6)$$

where

$$\hat{H}[\phi] = -\frac{\hbar^2}{2m^*}\frac{d^2}{d\phi^2} + V_0[\phi] + V_0 - \frac{F}{\omega_0^2}\phi\,, \qquad (7)$$

$m^* = (\hbar\omega_0 c_0/kT)^2$ and V_0 is a T-dependent energy offset. Equations (6) and (7) describe a quantum particle with coordinate ϕ and mass m^* confined to the asymmetric double-well $V_0[\phi] + V_0$ and subjected to the additional stopping tilt F/ω_0^2. Assume now that the two potential wells centered at $\phi_{1,2}$ may be approximated to nonoverlapping parabolic wells with curvature $\omega_{1,2}^2$, respectively. The difference between the lowest eigenvalues in the two

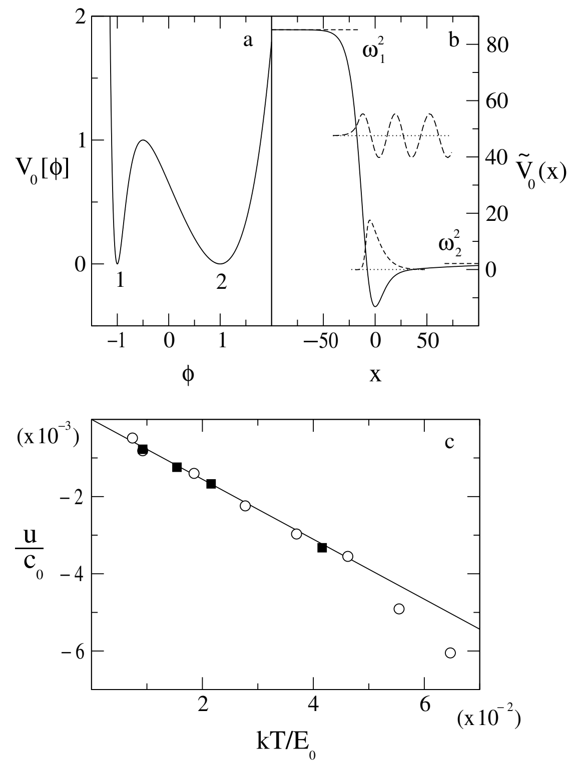

FIG. 2. (a) The ADW potential (12) with $\omega_0 = 1$, $b_1 = 0.5$, and $b_2 = 5.0$. Correspondingly, $\phi_{1,2} = \mp 1$, $\phi_0 = -0.50$, $\omega_1 = 9.23$, and $\omega_2 = 1.46$; (b) The relevant potential $\tilde{V}_0(x)$ of the stability equation (5). The Goldstone mode and a reflected phonon with $\omega_2 < \omega_k < \omega_1$ and $c_0 = 30$ are drawn for reader convenience (dashed curves). (c) The average ϕ_{12} speed u (in units of c_0) versus kT (in units of $E_0 = 1.80c_0\omega_0$) for $\alpha = 50$ and $c_0 = 60$ (circles) or $c_0 = 90$ (squares). All the remaining parameter values are as in (a). The solid line represents the temperature dependence predicted in (11).

parabolas vanishes under the following condition for the stopping tilt

$$\frac{aF}{\omega_0^2} = \frac{\hbar}{2\sqrt{m^*}}\left(\sqrt{V_0''[\phi_2]} - \sqrt{V_0''[\phi_1]}\right)$$
$$= -\frac{kT}{2c_0\omega_0}\frac{\omega_1 - \omega_2}{\omega_0}\,. \qquad (8)$$

As a consequence, the internal asymmetry effects on the soliton dynamics are equivalent to those produced by an external tilt $F_{\rm th}$ with intensity

$$aF_{\rm th} = \frac{kT}{2d}\frac{\Delta\omega}{\omega_0}\,. \qquad (9)$$

From the perturbation approach of Refs. [1,2] we conclude that a *tilted* asymmetric ϕ_{12} (or ϕ_{21}) undergoes Brownian motion with Langevin equation (LE)

$$M_0\ddot{X} = -\alpha M_0\dot{X} \mp (\Delta\epsilon + aF_{\rm th}) + \xi(t)\,, \qquad (10)$$

where M_0 is the soliton mass, $X(t)$ is the coordinate of its center of mass, and $\xi(t)$ is a Gaussian noise source with zero mean and autocorrelation function $\langle\xi(t)\xi(0)\rangle = 2\alpha M_0 kT\delta(t)$. In the zero tilt case, $\Delta\epsilon = 0$, the thermal force $\mp aF_{\rm th}$ drives the kink (antikink) to the left (right) with stationary speed $u_{\rm th}$,

$$\frac{u_{\rm th}}{c_0} = \mp \frac{kT}{2E_0}\frac{\Delta\omega}{\alpha}, \tag{11}$$

independent of c_0—being $E_0 \propto c_0\omega_0$, see Eq. (4).

We summarize now the limitations implicit in our derivation of (9)–(11): (i) kinks and antikinks have been treated in the dilute gas approximation, $kT \ll E_0$, that is imposing low soliton densities $n_0(T) \ll d^{-1}$ and nonrelativistic speeds $\langle u^2\rangle \ll c_0^2$ [7,9]; (ii) the stopping tilt F should not affect much the curvature of the minima of the tilted potential $\omega_0^2 V_0[\phi] - F\phi$, i.e., $|aF| \ll \omega_0^2$ or, for Eq. (9) to apply, $\Delta\omega/\omega_0 \ll c_0\omega_0/kT$; (iii) the smaller energy quantum $\hbar\omega_2$ of parabola 2 (we agreed to take $\Delta\omega \geq 0$) must be larger than the tunnel-splitting energy $\epsilon_1 - \epsilon_0$ in Eq. (6), that is $\omega_2/\omega_0 \gg dn_0(T)$ [6,8]; (iv) the soliton force $\mp aF_{\rm th}$ has been computed under the stronger assumption that the distance between valleys 1 and 2 of the tilted potential may be approximated to the unperturbed value a, i.e., $\omega_{1,2} \gtrsim \omega_0$.

For a quantitative comparison with the theory above we simulated Eqs. (1) and (2) for the asymmetric double-well (ADW) potential of Ref. [5]:

$$\omega_0^2 V_0[\phi] = \left(\frac{1 - \exp[b_1(\phi - 1)]}{1 - \exp[b_1(\phi_0 - 1)]} \times \frac{1 - \exp[-b_2(\phi + 1)]}{1 - \exp[-b_2(\phi_0 + 1)]}\right)^2. \tag{12}$$

The minima of $V_0[\phi]$ are located at $\phi_{1,2} = \pm 1$, its barrier is $\omega_0^2 = 1$ high and centered at $\phi = \phi_0$ (see caption of Fig. 2). Our simulation code is a framework based on Numerical Python and custom C libraries; time integration is performed by means of a modified Mil'shtein algorithm (see caption of Fig. 3 and Ref. [9]).

The kink center of mass $X(t)$, defined by $\phi_{12}(X,t) \equiv \phi_0$, is expected to fluctuate according to the LE (10) with $\Delta\epsilon = 0$. The average kink velocity $u \equiv \langle \dot{x}\rangle$ is plotted in Fig. 2(c) as a function of the temperature: Our simulation data are closely reproduced by law (11). It should be noticed that in the LE (10) temperature enters not only the random force $\xi(t)$, as customary in the theory of Brownian motion, but also the drift force $\mp aF_{\rm th}$. This effect (not to be mistaken for a solitonic ratchet [10]) is *entropic* in its nature, reflecting the tendency of the string to occupy the potential valley 2, where it may access the maximally disordered configurations compatible with its equilibrium temperature.

We are now in the position to answer the initial question about the direction of kink propagation in the tilted ADW potential of Fig. 1, chosen for convenience of the form

$$\omega_0^2 V[\phi] = \omega_0^2 V_0[\phi] + F_V\phi, \tag{13}$$

with $V_0[\phi]$ given in Eq. (12). The tilt in Eq. (13) tends to push ϕ_{12} to the right with constant driving force $\Delta\epsilon \simeq aF_V$, whereas the internal asymmetry of the ADW potential exerts on ϕ_{12} a force (9) to the left proportional to kT. The two mechanisms are expected to balance one another at a *critical* temperature T_c, such that

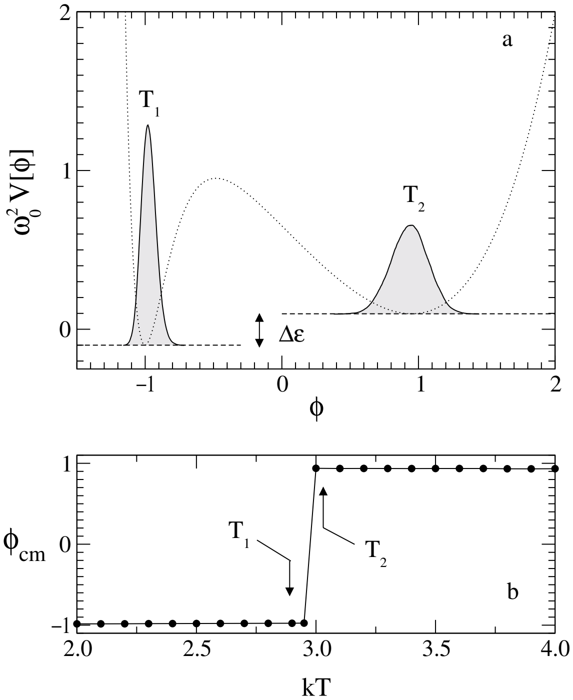

FIG. 3. (a) Normalized string distributions (solid curves) for $T_1 < T_c$ and $T_2 > T_c$ (arbitrary units) in the tilted ADW potential (13) with $F = 0.1$ (dotted line) and $V_0[\phi]$ plotted in Fig. 2(a); (b) String center of mass $\phi_{\rm cm}$ versus kT for the potential in (a) (integration step $\Delta t = 5 \times 10^{-3}$, string length $N = 10^4$, lattice constant $\Delta x = 1$, see text for details).

$$kT_c = 2d\Delta\epsilon\left(\frac{\omega_0}{\Delta\omega}\right). \tag{14}$$

We investigated such a temperature controlled *configurational transition* by simulating the relaxation of a string initially distributed at random between valleys 1 and 2: The corresponding kinks (antikinks), no matter how numerous, drift to the right (left) for $T < T_c$ and vice versa for $T > T_c$; independently of the initial conditions, the string eventually collapses into one valley as shown in Fig. 3(a). Such a transition is indeed very sharp; the critical temperature T_c can be determined numerically with an accuracy that increases with the length of the simulation runs. After 10^8 integration steps, our simulation yields $kT_c = 2.95 \div 3.00$ to compare with the estimate $kT_c \simeq 3.05$ obtained from prediction (14) [see Fig. 3(b)].

Thermal forces may affect the stability properties of the asymmetric deformable periodic (ADP) potentials, too (see the example of Fig. 4). The rich phenomenology of these double-well periodic potentials has been studied mostly numerically by many authors [4,11] (for a review, see Ref. [3]). In the absence of fluctuations *stable* kinks are those connecting two adjacent valleys 1 by crossing the enclosed valley 2; hence the notation ϕ_{121} employed in

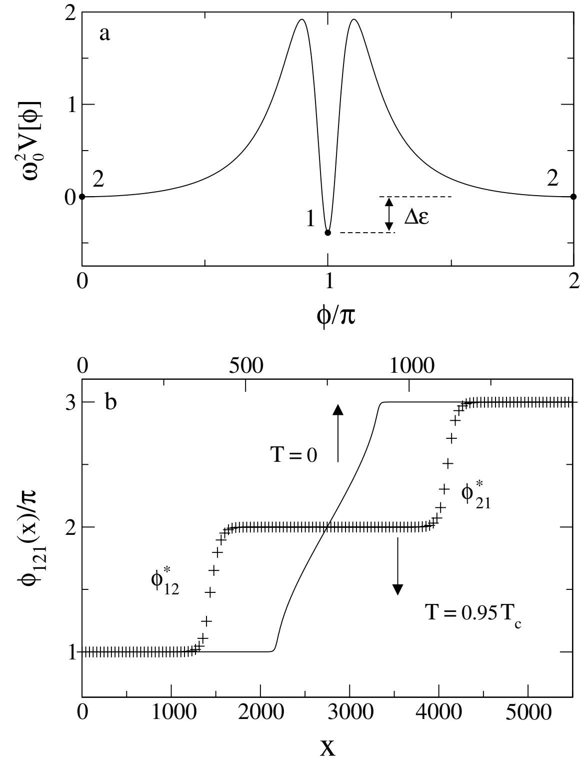

FIG. 4. (a) The ADP potential (15) for $A = 0.95$ and $B = 1.01$. The potential parameters are $\phi_1 = (2n + 1)\pi$ and $\phi_2 = 2n\pi$ with $n = 0, \pm 1, \ldots$, $\omega_0^2 = 2.31$, $\omega_1 = 13.13$, $\omega_2 = 0.32$, and $\Delta\epsilon = 0.39$; (b) Double kink ϕ_{121} at zero temperature (solid curve) and close to the dissociation point for $c_0 = 60$ (crosses). The latter has been computed by averaging the string configuration over time at $T = 0.95T_c$ (100 subsequent snapshots taken 10 time units apart). The expected value of kT_c is 3.65 to compare with the numerical estimate of 3.85 ± 0.05.

Fig. 4(b). A double kink ϕ_{121} may be regarded as a superposition of two *partials* ϕ_{12}^* and ϕ_{21}^*, both unstable against the drag due to the energy gap $\Delta\epsilon$: ϕ_{12}^* and ϕ_{21}^* drift towards one another (the former to the right, the latter to the left), thus making ϕ_{121} stable. Vice versa a kink ϕ_{212} connecting two adjacent valleys 2 is unstable. This exhausts the stability problem, e.g., of the double sine-Gordon string [11]. For the ADP potential [4]

$$\omega_0^2 V[\phi] = (1 - A^2)\,\frac{1 - B\cos 2\phi}{(1 + A\cos\phi)^2} \tag{15}$$

in Fig. 4(a), instead, the problem is complicated by the different curvatures $\omega_{1,2}$ of valleys 1 and 2 that, in view of our analysis, tend to pull ϕ_{12}^* and ϕ_{21}^* apart. A straightforward generalization of the argument leading to Eq. (14) allows us to determine the critical temperature above which the entropic forces acting upon the partials ϕ_{12}^* and ϕ_{21}^* overcome the binding force of ϕ_{121}, namely $kT_c = 2c_0(\Delta\epsilon/\Delta\omega)$. Above T_c the double kink ϕ_{121} is predicted to *dissociate* according to the action-mass law

$$\phi_{21}^* + \phi_{121} \rightarrow \phi_{212} + \phi_{21}^*, \tag{16}$$

with the objects on both sides being ordered from the left to the right as indicated and the partial ϕ_{21}^* traveling to the right throughout the reaction process. As T approaches T_c from below, the double kink ϕ_{121} gets broader and broader until for $T = T_c$ the partials ϕ_{12}^* and ϕ_{21}^* break loose [Fig. 4(b)]. As a result, for $T > T_c$ thermal fluctuations stabilize valleys 2 over valleys 1.

The mechanism of *stochastic stabilization* introduced here applies also to situations where fluctuations are fed in externally. This is the case, for instance, of the neuron cable model in neurophysiology, lately investigated by physicists [12] in the framework of stochastic resonance [13]. The string $\phi(x,t)$ is replaced by a chain of linearly coupled bistable oscillators of the type (12). The resulting array obeys a discretized version of the field equation (1), where $\zeta(x,t)$ is broken up into independent on-site noise sources $\zeta_i(t)$. Internal asymmetry, e.g., $\phi_0 \neq 0$ in an ADW chain (12), is likely to make the cable model much more interesting: (i) sustained by strong fluctuations, a signal can be transmitted in an otherwise less favorable direction (i.e., against an external voltage) according to a threshold mechanism; (ii) suprathreshold fluctuations are likely to fuel signal propagation more effectively than they garble it.

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