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Nucleation of Thermal Sine-Gordon Solitons: Effect of Many-Body Interactions

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The nucleation rate of *interacting* thermal kinks and antikinks in a sine-Gordon chain is evaluated within the dilute-gas approximation. Our novel result describes both the diffusive and nondiffusive limits. In comparison with the nondiffusive and noninteracting nucleation rate calculated previously by Büttiker and Landauer, interactions modify the temperature dependence of the prefactor and, in the diffusive limit, the Arrhenius factor as well.

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Condensed-matter physics, nonlinear optics, and engineering sciences provide a true storehouse of solitons.[1] In this paper we belabor the ubiquitous problem of transport of infinitely many particles in an array with infinitely many states of local stability, typified by a driven, damped sine-Gordon string. Such systems are investigated in connection with dislocation theory, charge-density waves in dielectrics, or Josephson transmission lines to name but a few.[1] Here, we consider the perturbed sine-Gordon equation for the field $\theta(x,t)$ in the units of moment of inertia[2] $I=1$,

$$\theta_{tt}+\alpha\theta_t=u_s^2\theta_{xx}-V_0\sin\theta-F+\xi(x,t), \tag{1}$$

where α is a friction coefficient, F a constant bias force, and u_s the sound velocity of the free string, and $\xi(x,t)$ denotes thermal, Gaussian white noise obeying at temperature T the Einstein relation

$$\langle\xi(x,t)\xi(x',t')\rangle=2\alpha kT\delta(t-t')\delta(x-x'). \tag{2}$$

Our principal interest is in the evaluation of the steady-state production rate of kink-antikink pairs. Nucleation of pairs does not modify the *winding* number of the sine-Gordon string.[3,4] Our determination of the nucleation rate is, therefore, independent of the total topological charge of the string. The presence of the fluctuating force $\xi(x,t)$ impacts the transport properties of the thermalized gas of kinks and antikinks. These kink-antikink collisions can be analyzed by extension of the perturbation treatment[3] of McLaughlin and Scott.[4] The collision of two unperturbed kinks (or antikinks) is elastic with a mutual repulsive interaction. With the friction force acting this bouncing mechanism is essentially unchanged. The situation is markedly distinct, however, for kink-antikink collisions. The kink-antikink interaction is attractive and, in the absence of thermal forces, reflectionless. This is no longer true in the presence of a strong damping. The internal viscosity[4] of the colliding kink-antikink string configuration may not be compensated by an external field of limited strength or by weak thermal fluctuations; i.e., the kink-antikink collision becomes *destructive* provided that[5]

$$F/V_0<F^{\rm th}/V_0\equiv 2(\alpha/\omega_0)^{3/2}, \tag{3}$$

with $V_0\equiv\omega_0^2$. In the following we shall address only the overdamped limit, $\alpha\gg\omega_0$, so that in the region of multistability ($F/V_0<1$) the condition (3) is always satisfied.

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In the overdamped limit the propagation velocity u_F of a driven kink exhibits a universal behavior[2,6]

$$u_F = u_0 \phi(F/V_0), \tag{4}$$

where $u_0 = u_s \omega_0/\alpha$, and ϕ is a universal function. For small fields, say $F/V_0 < 0.5$, ϕ is to excellent approximation linear in F, i.e.,

$$u_F = u_0 \tfrac{1}{4} \pi F/V_0. \tag{5}$$

With $\alpha \gg \omega_0$, relativistic corrections to u_F do not enter.[6] The motion of a single kink solution obeys a driven Langevin dynamics.[3] On introducing the kink momentum $p \equiv (u/u_s)E_0(1-u^2/u_s^2)^{-1/2}$, with $u = \dot{x}$, and making use of the perturbation argument of Ref. 4, one obtains the relativistic Langevin equation driven by Gaussian white noise, $\gamma(t)$, of vanishing mean,[7,8]

$$\dot{p} = -\alpha p + \alpha(u_0/u_s)E_0\phi(F/V_0) + \sqrt{E_0}\gamma(t). \tag{6}$$

Here $\gamma(t)$ obeys the Einstein relation $\langle\gamma(t)\gamma(0)\rangle = 2\alpha k \times T\delta(t)$, and $E_0 = 8u_s\omega_0$ denotes the rest energy of an unperturbed (anti)kink. In the overdamped (and, therefore, nonrelativistic) limit we obtain from (6) the Langevin equation of motion for the kink center of mass,

$$\dot{x} = u_F + \zeta(t), \tag{7}$$

where $\langle\zeta(t)\zeta(0)\rangle = 2D\delta(t)$, with $D = (kT/\alpha E_0)u_s^2$.

We now turn to the problem of nucleation of kink-antikink pairs in the *presence* of a dilute gas of thermalized kinks and antikinks. Previously, the problem of nucleation has been addressed[2,9] under the condition that many-body effects due to the presence of other kinks are negligible. In this case, Büttiker and Landauer[2] (see also Pokrovskii and co-workers[9]) invoke Langer's approach[10] to calculate the "escape" of a sine-Gordon string through a bias-dependent saddle-point configuration (critical nucleus) corresponding to an energy barrier $2E_F$. Their results are valid within the limit of a dilute gas ($E_F \gg kT$) and large bias forces. The latter condition implies that the width of the critical nucleus is small and the diffusive motion of its components [see (7)] can be safely neglected. The treatment in Ref. 2 can be pictured as the escape of a single "particle" (corresponding to the relative coordinate of the nucleating partners) over a potential barrier $2E_F$ into the vacuum[11,12]; such a particle is not allowed to collide with the gas of thermalized kinks (antikinks) during the process of nucleation. Thus, this treatment does not account for the many-body effects, such as a finite lifetime, which other thermalized pairs may impose on the critical nucleus.

In order to evaluate the production rate in the presence of such many-body interactions, we rely on the statistical mechanics for a dilute gas of kink-antikink pairs. The mean square displacement of a single (anti)kink follows from (7), i.e.,

$$\langle\Delta x^2(t)\rangle = 2Dt + u_F^2 t^2 - 2D(1-e^{-\alpha t})/\alpha. \tag{8}$$

Since the average distance L between annihilating (anti)kinks is given by $L = 1/n_0$, where n_0 denotes the steady-state kink density, the mean lifetime τ_F of kinks in the dilute-gas approximation is determined by the identities $\langle\Delta x^2(\tau_F)\rangle = L^2 = n_0^{-2}$. Observing that in the overdamped regime the third term on the right-hand side of (8) is negligible, we obtain

$$\tau_F = (D/u_F^2)\{-1 + [1 + (u_F/Dn_0)^2]^{1/2}\}, \tag{9}$$

valid *in both the diffusive and nondiffusive regimes of kink propagation.*

The *diffusive* limit is characterized by the condition $u_F \ll Dn_0$; see (7) and (9). In other words, with $u_F < u_s$ the diffusive limit implies extremely small fields $F \ll F_c \equiv kTn_0/2\pi$. Thus, with the dilute-gas limit (i.e., $kTn_0/V_0 \ll 1$) one finds for the lifetime in the diffusive limit

$$\tau_F \to \tau_D = (2Dn_0^2)^{-1}, \quad F \ll F_c. \tag{10}$$

Likewise, the *nondiffusive* limit yields

$$\tau_F \to \tau_0 = (u_F n_0)^{-1}, \quad F \gg F_c. \tag{11}$$

The production rate Γ of thermal kink-antikink pairs over unit length is thus given by the ratio of twice the steady-state kink density over the kink mean lifetime, i.e.,

$$\Gamma = 2n_0/\tau_F = 2n_0^3 D\{[1 + (F/F_c)^2]^{1/2} + 1\}. \tag{12}$$

This is the main result of this paper. It describes a smooth *crossover* between the diffusion-controlled production rate Γ_D and the nondiffusive limit Γ_0. The two limits of (12) read

$$\Gamma_D = 4Dn_0^3, \quad F \ll F_c, \tag{13}$$

and

$$\Gamma_0 = 2u_F n_0^2, \quad F \gg F_c. \tag{14}$$

The general expression for Γ, (12), as well as the limiting results (13) and (14), are given in terms of the steady-state density n_0 at finite bias F. To evaluate n_0 in the bias dominated regime we can invoke Langer's procedure[10] which relates the nucleation rate to the imaginary part of the free energy of the critical nucleus, $\mathrm{Im}\mathcal{F}$, i.e.,

$$\Gamma_0 = (|\lambda^N|/\pi kT)\mathrm{Im}\mathcal{F}, \quad F \gg F_c. \tag{15}$$

The condition $F \gg F_c$ implies that the nucleating kink and antikink gain an energy much larger than kT moving away from each other prior to subsequent annihilation, and, thus, they do not strongly interact with other nucleating pairs during the creation process. λ^N denotes the negative eigenvalue which corresponds to the saddle-point configuration of the nucleus. We determined λ^N for $F/V_0 < \frac{1}{2}$ analytically:[8]

$$\lambda^N = -\tfrac{1}{2}\pi F/\alpha. \tag{16}$$

At strong fields, $kT/E_0 < F/V_0 < 1$, λ^N is well separated from the zero mode (Goldstone mode) describing the translational invariance of the nucleation process. In this case, $\mathrm{Im}\mathcal{F}$ can be evaluated within the vicinity of the saddle point and an alternative determination of Γ_0 is obtained [see Eq. (21)]. Following Ref. 2 we denote the result for the nucleation rate in this strong-field limit by $\Gamma_0 \equiv \Gamma_{BL}$. This in turn yields for the steady-state density $n_0 = (\Gamma_{BL}/2u_F)^{1/2}$. Next we consider the case of weak forces, F being so small that the mechanical energy required for pulling an isolated kink through a distance of the size of its width u_s/ω_0 is less than the thermal energy, kT, stored in the nucleating pair, i.e., $2\pi F(u_s/\omega_0) < kT$ or, equivalently, $\frac{1}{4}\pi F/V_0 < kT/E_0$. With $F/V_0 < kT/E_0$ the nucleus configuration attains a broad extension. In this regime we can describe the nucleus as a linear superposition of a kink and an antikink separated by a distance X and whose interaction is mediated by the effective potential[9]

$$U(X) = 2E_0 - 2\pi F X - 4E_0 \exp(-\omega_0 X/u_s).$$

The width X_c of the critical nucleus is given by $U'(X_c) = 0$, i.e., $X_c = (u_s/\omega_0)\ln(16\omega_0^2/\pi F)$. $U(X_c)$ provides a good estimate of the nucleation energy $2E_F$. Taking further into account effects due to the change of the kink shape with varying the nucleus width, we obtained[8] an improved, and rather accurate result for $2E_F$, i.e.,

$$2E_F = U(X_c) - \frac{\pi}{8}\frac{F}{V_0}E_0 = 2E_0\left\{1 + \frac{\pi}{8}\frac{F}{V_0}\left[\ln\left(\frac{\pi F}{16 V_0}\right) - 1\right]\right\}, \quad \frac{F}{V_0} < 0.9. \tag{17}$$

With $F/V_0 < kT/E_0$ the potential barrier $U(X)$ about X_c is very flat and E_F can be identified to a good approximation with the *rest energy* of a driven kink. Use of the same arguments as in thermal equilibrium (see, e.g., Appendix C in Ref. 2) then yields for the steady-state density at weak forces

$$n_0 = (2/\pi)^{1/2}(\omega_0/u_s)(E_F/kT)^{1/2}\exp(-E_F/kT), \quad F/V_0 < kT/E_0. \tag{18}$$

This very result can be checked by our calculating alternatively Γ_0 from (15) with the restriction $F_c/V_0 \ll F/V_0 < kT/E_0$ and, then, making use of the identity in (14), i.e., $n_0 = (\Gamma_0/2u_F)^{1/2}$. In such a regime the approximations[10,11] leading to Γ_{BL} do not apply, because one has to deal with *two* coupled collective coordinates, the Goldstone mode and a "breathing mode."[13] The latter mode describes fluctuations that change the relative separation between the kink-antikink components of the extended nucleus configuration, but leave the nucleation energy essentially unchanged. It is characterized by a small negative eigenvalue [see (16)]. Following the recipe presented in Ref. 13, one obtains Γ_0 and, through (14), again (18). For F tending to zero, n_0 approaches the well-known thermal equilibrium density,[1,2] $n_0(F=0) = n_{eq}$. Insertion of (18) in (12) yields an explicit expression for the production-rate formula which interpolates, now, between Γ_D and Γ_0 with $F/V_0 < kT/E_0$.

The new explicit result for Γ_D valid at vanishingly small forces, $F \ll F_c$, reads

$$\Gamma_D = (2/\pi)^{3/2}(\omega_0/u_s)^2(E_F/2\alpha)(E_F/kT)^{1/2}\exp(-3E_F/kT). \tag{19}$$

For $F = 0$, this special result has been obtained (apart from an incorrect constant in the prefactor) by one of us previously.[14] Note that the Arrhenius factor involves 3 times the rest energy of a driven kink, and the prefactor exhibits a universal $T^{-1/2}$ dependence.

On inserting (5) and (18) in (14), we obtain an approximate expression for Γ_0, i.e.,

$$\Gamma_0 = (\omega_0/u_s)(F/\alpha)(E_F/kT)\exp(-2E_F/kT), \quad F_c/V_0 \ll F/V_0 < kT/E_0. \tag{20}$$

Here, the presence of thermalized kinks during nucleation does not affect the Arrhenius factor of the production-rate formula but only its prefactor, which exhibits a universal inverse dependence on the temperature. In fact, the Büttiker and Landauer prediction for the production rate in this regime[2,9] can be written explicitly as[8]

$$\Gamma_{BL} = \frac{1}{\pi\alpha}\left(\frac{\omega_0^2}{u_s}\right)(2F)^{1/2}\left(\frac{E_F}{kT}\right)^{1/2}\exp\left(\frac{-2E_F}{kT}\right). \tag{21}$$

This result, being a valid expression for moderately strong forces $kT/E_0 < F/V_0 < \frac{1}{2}$, differs from (20) by a finite-lifetime-induced renormalization of the damping coefficient α (i.e., a breathing-mode renormalization),[15]

$$\alpha \to \alpha_{BL} = \alpha\frac{\omega_0}{\pi}\left(\frac{2}{F}\right)^{1/2}\left(\frac{kT}{E_F}\right)^{1/2}. \tag{22}$$

In conclusion, we have presented a unique approach to the nucleation rate of thermalized kink-antikink pairs in the limit of a dilute gas ($kT/E_F \ll 1$) by taking explicitly into account the effective interaction with other present thermalized kink (antikink) solutions. These physically important many-kink effects have not been addressed previously in studies of the nucleation of kink-antikink pairs.[2,9] Our results are valid in the overdamped limit ($\alpha \gg \omega_0$) thereby assuring that kink-antikink collisions are always destructive. We have addressed both the diffusive and the nondiffusive regimes of kink propagation and found a smooth crossover between these limits in terms of the mean lifetime τ_F in (9). The interaction always affects the prefactor of the nucleation rate. Moreover, in the diffusive regime it also has a strong effect on the Arrhenius factor with a smooth crossover from 3 times the rest energy of a kink to a value given by $2E_F$ [see (17)].

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