A Langevin Equation Approach to Sine-Gordon Soliton Diffusion with Application to Nucleation Rates

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1. Introduction

The sine-Gordon (SG) equation (in units of the speed of light c = 1)

$$\phi_{tt} - \phi_{xx} + m^2 \sin\phi = 0 \tag{1}$$

bears both standing-wave (phonons) and solitary-wave solutions (solitons). Equation (1) can be derived from the relativistically covariant Hamiltonian density $H[\phi] = \frac{1}{2}(\phi_x^2 + \phi_t^2) - m^2\cos\phi$, m being a lattice constant(1). For later convenience, we write explicitly the *single* soliton solution (mod 2π)

$$\phi^{K;\bar{K}}(x,u) = 4\,\mathrm{tg}^{-1}\left\{\exp\left[\pm m\gamma(x - X(t))\right]\right\}, \quad X(t) = x_0 + ut \ . \tag{2}$$

Here, ± signs refer to the two possible helicities of the solution (kink ϕ^K and anti-kink $\phi^{\bar{K}}$, respectively), $\gamma \equiv (1 - u^2)^{-1/2}$ denotes the Lorentz contraction and *u* the translational speed of the soliton. $\phi^{K;\bar{K}}$ carry opposite topological charge and are stable against almost every small fluctuation, the only exception being a rigid translation, against which $\phi^{K;\bar{K}}$ are in neutral equilibrium (Goldstone mode).

The statistical SG theory deals with a gas of phonons and solitons, the number of which is controlled by the relevant creation energy (or chemical potential in the grand-canonical formalism). A statistical mechanical approach has been proposed by Currie *et al.*(2) for the limit of low temperature, where solitary waves may be approximated to a linear superposition of non-interacting kinks (K) and antikinks ($\bar{K}$) (dilute gas approximation). The creation (or rest) energy for $\phi^{K;\bar{K}}$ is given by the integral $E_0 = \int dx\, H[\phi^{K;\bar{K}}(x,0)] = 8m$, whence the low temperature condition(2) $\beta E_0 >> 1$, $\beta \equiv (kT)^{-1}$ being the reciprocal of the absolute temperature. The mean square velocity of $\phi^{K;\bar{K}}$ coincides with the gas kinetic theory prediction $(\beta E_0)^{-1}$.

The equilibrium kink-density per unit of length, n_0, is defined as the ratio between the (canonical) partition function of the field configurations with one soliton, and the partition function with no soliton present(1,3)

$$n_0 = \left(\frac{2}{\pi}\right)^{1/2} m(\beta E_0)^{1/2}\, e^{-\beta E_0} \ . \tag{3}$$

The (canonical) partition functions of the statistical SG theory at a given temperature, can be obtained through the stationary statistics of the stochastic process(4)

$$\phi_{tt} - \phi_{xx} + m^2 \sin\phi = - \alpha\, \phi_t + \zeta(x, t) \quad , \tag{4}$$

where $\zeta(x, t)$ is a Gaussian fluctuating field of force with $<\zeta> = 0$ and $<\zeta(x, t)\, \zeta(x', t')> = 2\alpha kT\, \delta(t - t')\, \delta(x - x')$. In the presence of *small* fluctuations, $\beta E_0 >> 1$, $\phi^{K;\bar{K}}$ is stable and undergoes Brownian motion[4-6].

2. The Langevin equation

For the sake of generality we add to the rhs of (4) a constant bias F, i.e.

$$\phi_{tt} - \phi_{xx} + m^2 \sin\phi = - \alpha\, \phi_t - F + \zeta(x, t) \quad . \tag{5}$$

The condition $F < m^2$ is imposed to preserve the multistability of the system. Following the perturbation approach of Ref. 7 we assume that in the zero-th order the shape of the single kink solution (2) is left unchanged, whereas the perturbation on the rhs of (5) only affects the motion of the coordinates $X(t)$ and $u(t) \equiv \dot{X}(t)$. Thus, on invoking a simple energy conservation argument[7],

$$\frac{d}{dt}\int dx\, H[\phi^{K;\bar{K}}(x, u(t))] \equiv E_0 \frac{d}{dt}\gamma(t) = - \int dx[\alpha\, \phi_t^{K;\bar{K}} + F - \zeta(x, t)]\, \phi_t^{K;\bar{K}} , \tag{6}$$

where $\gamma(t) = (1 - u^2(t))^{-1/2}$ is the stochastic Lorentz contraction, we obtain the following relativistic Langevin equation (LE)[8]

$$\dot{p} = - \alpha p + 2\pi F + \gamma(t) E_0\, \xi(t) \quad . \tag{7}$$

$\xi(t)$ is a Gaussian fluctuating force with $<\xi> = 0$ and $<\xi(t)\, \xi(0)> = 2\alpha[\gamma(t)\beta E_0]^{-1}\, \delta(t)$. $p(t)$ denotes here the momentum of $\phi^{K;\bar{K}}$, i.e. $p(t) = \gamma(t)\, E_0\, u(t)$.

The LE (7) holds for any value of the frictional constant α. However, in view of application to overdamped systems - but losing generality - we impose the condition $\alpha >> m$. In the overdamped limit three major simplifications are allowed: (i) time-dependent solutions to (1), e.g. breathers, are damped and, therefore, do not play any significant role in the statistics of the problem[3,7]; (ii) our results can be worked out in the non-relativistic approximation $\gamma \to 1$; (iii) K-$\bar{K}$ collisions are almost always destructive[7], i.e. the relevant transmission coefficient is exponentially small. In the limit $\gamma \to 1$, (7) reads

$$\dot{u} = - \alpha u + \frac{\pi}{4}\frac{F}{m} + \xi(t) \quad . \tag{8}$$

In the absence of fluctuations the translational speed of $\phi^{K;\bar{K}}$ approaches a stationary value inversely proportional to α, i.e.

$$u_F = \pm \frac{\pi}{4}\frac{F}{m\alpha} \quad . \tag{9}$$

Moreover, the fluctuations about u_F are very small at low temperature, i.e. $<(u(t) - u_F)^2> \cong (\beta E_0)^{-1}$, thus justifying the non-relativistic approximation.

3. Nucleation rates

a) Nucleation of a single K-$\bar{K}$ pair[1,3,9].

Thermal kinks and antikinks are produced in pairs so that the total topological charge of the system is conserved.Thermal fluctuations trigger the process by activating a large nucleus about a vacuum configuration of the field ϕ, say $\phi_0 = 0$. Such a nucleus is described by the doublet-solution[3] $\phi_D = 4tg^{-1}[sh(mu\gamma t) / u\ ch\ (m\gamma x)]$ (the origin of x and t are taken arbitrary) and when its size grows very large it can be approximated by a linear superposition of a kink and an antikink.The components of a large nucleus ϕ_D experience two contrasting forces, an *attractive* force due to the vicinity of the nucleating partner, the potential of interaction being a function of the distance 2X between their centres of mass ,

$$V_D(X) = -2E_0\, e^{-2mX}, \qquad mX >> 1, \tag{10}$$

and a *repulsive* force due to the external bias F, which pulls ϕ^K and $\phi^{\bar{K}}$ apart.

Such a single-pair nucleation process can be described in our LE scheme by substituting ϕ_D in (6). This amounts to just adding a K$-\bar{K}$ interaction term in (7); for a nucleating *kink* we have (in ϕ_D rest frame)

$$\ddot{X} = -\alpha\dot{X} - 4m\, e^{-2mX} + \frac{\pi}{4}\frac{F}{m} + \xi(t) \quad . \tag{11}$$

The nucleation process is thus reduced to the problem of the stochastic decay of a one-dimensional metastable state. The relevant potential barrier is located at $X_p(F) = -(2m)^{-1}\ln(\pi F/16\, m^2)$ with curvature $|\Omega|^2 = \pi F/2$. Note that for $F << m^2$ the critical size of ϕ_D becomes much larger than the single soliton size m^{-1}.The activation energy $\Delta E(F)$ can be calculated by employing the same argument as in (6):

$$\frac{d}{dF}\Delta E(F) = -\int dx\, \phi_D(x) \equiv -2\pi\,(2X_p(F)) \quad . \tag{12}$$

On substituting the explicit expression for $X_p(F)$ and carrying out the integration with initial condition $\Delta E(0) = 2E_0$ (rest pair energy for $X_p \to \infty$) we obtain[8]

$$\Delta E(F) \equiv 2E_F = 2E_0\left(1 + \frac{\pi}{8}\frac{F}{m^2}\left[\ln\left(\frac{\pi}{16}\frac{F}{m^2}\right) - 1\right]\right) \quad . \tag{13}$$

The LE (11) only describes the stochastic decay of the unstable mode X(t), irrespective of the *stable modes* (phonons) dressing both the vacuum ϕ_0 and the pair configuration, $\phi_D(x) \equiv \phi^K(x-X) - \phi^{\bar{K}}(x+X)$. The decay rate of a metastable *multidimensional* system in the overdamped limit has been calculated by Langer[10]. Since in the present case there exist only one translational mode (the process is invariant under translation) and one metastable mode X(t) , Langer's formula is

$$\Gamma = \frac{1}{2\pi}\frac{|\Omega|^2}{\alpha^{1/2}}\left(\frac{\beta\Delta E}{2\pi}\right)^{1/2}\left\{\frac{\prod_n \lambda_n^0}{\prod_{n\neq 1} |\lambda_n^D|}\right\}^{1/2} e^{-\beta\Delta E} \quad . \tag{14}$$

The quantity in braces has been calculated explicitly by Langer[10] and Büttiker and Landauer (Appendix B of Ref. 3). Substituting the explicit expressions for the quantities appearing in (14) yields an *analytical* result for the Büttiker-Landauer nucleation rate[3], which reads[8]

$$\Gamma_{BL} = \frac{\sqrt{2}}{\pi} \frac{m^2\sqrt{F}}{\alpha} (\beta E_F)^{1/2} e^{-2\beta E_F} \quad . \tag{15}$$

An advantage of our approach compared with that of Ref. 3 is that it provides an analytical expression for the negative eigenvalue $\lambda_0^D = \Omega^2/\alpha = -\pi F/(2\alpha)$, which fits the numerical calculation[3] for $F < m^2/2$. Since $\Delta E(F)$, (13), reproduces the relevant numerical result of Ref. 3 for even larger values of F, our determination of Γ_{BL} holds eventually for $F < m^2/2$. An analytical expression for Γ_{BL} in the limit $F \rightarrow m^2$ is also available[3;9]. According to Büttiker and Landauer[3] the nucleation mechanism described above is only valid when the thermal energy kT is much smaller than the mechanical work done by the external force F in the (free) soliton lifetime, i.e. $2\pi F < n_0 kT$. It should be remarked, however, that for $F/m^2 < kT/E_0 << 1$ the nucleus has a broad width. Under such circumstances a Langer decay mechanism for the nucleus is no longer tenable. Moreover, effects due to the finite lifetime of a given thermal pair in the presence of a $K-\bar{K}$ gas are to play a decisive role[8,11].

b) Nucleation of interacting pairs[8]

A quite different prediction for the $K-\bar{K}$ nucleation rate in the overdamped limit may be obtained by equating the kink production rate to the annihilation rate. The calculation of the annihilation rate is very simple for $\alpha >> m$, where $K-\bar{K}$ collisions are always *destructive.*

The mean square displacement of a diffusive soliton follows from (8),

$$\langle \Delta X^2(t) \rangle = 2Dt + u_F^2 t^2 - \frac{2D}{\alpha}(1 - e^{-\alpha t}) \tag{16}$$

with $D = (\beta E_0 \alpha)^{-1}$. Observing that the average distance between annihilating solitons is given by $L = n_0^{-1}$, the soliton mean lifetime, τ_F, is determined by the equation $\langle \Delta X^2(\tau_F) \rangle = L^2$, i.e. in the dilute gas approximation,

$$\tau_F \cong \frac{D}{u_F^2}\left[-1 + \sqrt{1 + \left(\frac{u_F}{Dn_0}\right)^2} \right] \quad . \tag{17}$$

The production (annihilation) rate of thermal K-$\bar{K}$ pairs per length unit is thus given by the universal function[8]

$$\Gamma = \frac{2n_0}{\tau_F} = 2n_0^3 D \left[\sqrt{1 + \left(\frac{F}{F_c}\right)^2} + 1 \right] \quad , \tag{18}$$

where $F_c \equiv kT\, n_0 / 2\pi$. The steady-state kink density $n_0 \equiv n_0(F)$ has been worked out from the definition of n_0 given in the introduction when the presence of the external field is accounted for [8]. In the leading order $n_0(F)$ is given by (3) where in the exponential E_0 is replaced with E_F in (13).

Eq. (18) can be specialized to two important limits:

(i): Diffusive limit: $F << F_c$ in (18) implies $\Gamma_D \cong 4 D n_0^3$, and, explicitly[8,11]

$$\Gamma_D = m^2 \left(\frac{2}{\pi}\right)^{3/2} \frac{E_F}{2\alpha} (\beta E_F)^{1/2} \; e^{-3\beta E_F} \quad . \tag{19}$$

Note that the Arrhenius factor in (19) involves *three times* the rest energy of a soliton.

(ii) Ballistic limit: $F >> F_c$ in (18) justifies the approximation[8] $\Gamma_B \cong 2\, u_F\, n_0^2$, i.e.

$$\Gamma_B = m \,\frac{F}{\alpha}\, (\beta E_F)\, e^{-2\beta E_F} \qquad \left(\frac{F}{m^2} < \frac{kT}{E_0}\right) \quad . \tag{20}$$

The two results in (15) and (20) differ by an interaction induced renormalization of the damping coefficient α in (15) , $\alpha \rightarrow \alpha_{BL} = \alpha(m/\pi)\ (2/F\beta E_F)^{1/2}$. Compared with (15) the result in (20) exhibits an additional factor of $(\beta E_F)^{1/2}$, which amounts to the "breathing - mode" contribution, i.e. with $(F/m^2) < kT/E_0$, λ_0^D is a small negative eigenvalue which, in addition to the Goldstone mode, can be treated as an approximate, collective variable to be integrated over[12].

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