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# 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  $c = 1$ )

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

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<sup>(1)</sup>. For later convenience, we write explicitly the *single* soliton solution (mod  $2\pi$ )

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

Here,  $\pm$  signs refer to the two possible helicities of the solution (kink  $\phi^K$  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.*<sup>(2)</sup> 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<sup>(2)</sup>  $\beta E_0 \gg 1$ ,  $\beta \equiv (kT)^{-1}$  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<sup>(1,3)</sup>

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

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

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

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

## 2. The Langevin equation

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

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

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<sup>(7)</sup>,

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

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

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

$\xi(t)$  is a Gaussian fluctuating force with  $\langle \xi \rangle = 0$  and  $\langle \xi(t) \xi(0) \rangle = 2\alpha[\gamma(t)\beta E_0]^{-1} \delta(t)$ .  $p(t)$  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  $\alpha$ . However, in view of application to overdamped systems - but losing generality - we impose the condition  $\alpha \gg m$ . 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<sup>(3,7)</sup>; (ii) our results can be worked out in the non-relativistic approximation  $\gamma \rightarrow 1$ ; (iii)  $K-\bar{K}$  collisions are almost always destructive<sup>(7)</sup>, i.e. the relevant transmission coefficient is exponentially small. In the limit  $\gamma \rightarrow 1$ , (7) reads

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

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

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

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

### 3. Nucleation rates

#### a) Nucleation of a single K- $\bar{K}$ pair<sup>(1,3,9)</sup>.

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  $\phi$ , say  $\phi_0 = 0$ . Such a nucleus is described by the doublet-solution<sup>(3)</sup>  $\phi_D = 4\text{tg}^{-1}[\text{sh}(muyt) / u \text{ch}(myx)]$  (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  $\phi_D$  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 ,

$$V_D(X) = -2E_0 e^{-2mX}, \quad mX \gg 1, \quad (10)$$

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

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

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

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  $F \ll m^2$  the critical size of  $\phi_D$  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):

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

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  $X_p \rightarrow \infty$ ) we obtain<sup>(8)</sup>

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

The LE (11) only describes the stochastic decay of the unstable mode  $X(t)$ , irrespective of the *stable modes* (phonons) dressing both the vacuum  $\phi_0$  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<sup>(10)</sup>. 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

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

The quantity in braces has been calculated explicitly by Langer<sup>(10)</sup> 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<sup>(3)</sup>, which reads<sup>(8)</sup>

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

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<sup>(3)</sup> 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  $\Gamma_{BL}$  holds eventually for  $F < m^2/2$ . An analytical expression for  $\Gamma_{BL}$  in the limit  $F \rightarrow m^2$  is also available<sup>(3;9)</sup>. According to Büttiker and Landauer<sup>(3)</sup> 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  $F/m^2 < kT/E_0 \ll 1$  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<sup>(8,11)</sup>.

#### b) Nucleation of interacting pairs<sup>(8)</sup>

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  $\alpha \gg m$ , where  $K-\bar{K}$  collisions are always *destructive*.

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

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

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,  $\tau_F$ , is determined by the equation  $\langle \Delta X^2(\tau_F) \rangle = L^2$ , i.e. in the dilute gas approximation,

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

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

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

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<sup>(8)</sup>. 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:  $F \ll F_c$  in (18) implies  $\Gamma_D \cong 4 D n_0^3$ , and, explicitly<sup>(8,11)</sup>

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

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

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

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

The two results in (15) and (20) differ by an interaction induced renormalization of the damping coefficient  $\alpha$  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  $(F/m^2) < kT/E_0$ ,  $\lambda_0^D$  is a small negative eigenvalue which, in addition to the Goldstone mode, can be treated as an approximate, collective variable to be integrated over<sup>(12)</sup>.

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