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 \(c = 1\))

\[
\phi_t - \phi_{xx} + m^2 \sin \phi = 0 \tag{1}
\]

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\(^{1(1)}\). For later convenience, we write explicitly the single soliton solution (mod \(2\pi\))

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

Here, \(\pm\) signs refer to the two possible helicities of the solution (kink \(\phi^K\) and anti-kink \(\phi^-\), respectively), \(\gamma = (1 - u^2)^{-1/2}\) denotes the Lorentz contraction and \(u\) the translational speed of the soliton. \(\phi^{K;R}\) carry opposite topological charge and are stable against almost every small fluctuation, the only exception being a rigid translation, against which \(\phi^{K;R}\) 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 \textit{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\(^{(2)}\)

\[
\beta E_0 >> 1, \quad \beta \equiv (k T)^{-1} \text{ being the reciprocal of the absolute temperature. The mean square velocity of } \phi^{K;\bar{K}} \text{ coincides with the gas kinetic theory prediction } (\beta E_0)^{-1}.
\]

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

(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, \( \beta E_0 >> 1 \), \( \phi^{K:\bar{K}} \) 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.

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

(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\(^{(7)}\),

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

(6)

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

\[ \dot{p} = - \alpha p + 2\pi F + \gamma(t)E_0 \xi(t). \]  

(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. \( p(t) = \gamma(t)E_0u(t) \).

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 \( \alpha >> m \). 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 \( \gamma \rightarrow 1 \); (iii) \( K-\bar{K} \) collisions are almost always destructive\(^{(7)}\), i.e. the relevant transmission coefficient is exponentially small. In the limit \( \gamma \rightarrow 1 \), (7) reads

\[ \dot{u} = - \alpha u + \frac{\pi}{4} \frac{F}{m} + \xi(t). \]  

(8)

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

\[ u_F = \pm \frac{\pi}{4} \frac{F}{m\alpha}. \]  

(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–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 \(\phi\), say \(\phi_0 = 0\). Such a nucleus is described by the doublet-solution\(^{(3)}\) \(\phi_D = 4t \exp[-\text{sh}(m\chi t)] / \sqrt{\text{ch}(m\chi t)}\) (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 \textit{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 \textit{repulsive} force due to the external bias \(F\), which pulls \(\phi^K\) and \(\phi^\overline{K}\) 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 \(K–\overline{K}\) interaction term in (7); for a nucleating \textit{kink} we have (in \(\phi_D\) rest frame)

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

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 \(X_p(F) = -(2m)^{-1} \ln(\pi F/16 \text{ m}^2)\) with curvature \(\Omega^2 = \pi F/2\). Note that for \(F \ll \text{m}^2\) 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):

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

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 \(X_p \to \infty\)) we obtain\(^{(8)}\)

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

The LE (11) only describes the stochastic decay of the unstable mode \(X(t)\), irrespective of the \textit{stable modes} (phonons) dressing both the vacuum \(\phi_0\) and the pair configuration, \(\phi_D(x) = \phi^K (x–X) – \phi^\overline{K} (x + X)\). The decay rate of a metastable \textit{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

\[
\Gamma = \frac{1}{2\pi \alpha^{1/2}} \left(\frac{\beta^2}{2\pi} \right)^{1/2} \left\{ \prod_{n \neq 1} \lambda_n^{0} \left| \lambda_n^D \right| \right\}^{1/2} e^{-\beta \Delta E} \quad (14)
\]
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\(^{8}\)

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

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 \(\Gamma_{\text{BL}}\) holds eventually for \(F < m^2/2\). An analytical expression for \(\Gamma_{\text{BL}}\) 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. \(2\pi F < n_0^2 kT\). 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 \(K^+\overline{K}\) gas are to play a decisive role\(^{8,11}\).

b) Nucleation of interacting pairs\(^8\)

A quite different prediction for the \(K^+\overline{K}\) 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 \(K^+\overline{K}\) collisions are always destructive.

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

\[
\langle \Delta X^2(t) \rangle = 2D t + u_F^2 t^2 - \frac{2D}{\alpha} (1 - e^{-\alpha t})
\]  

(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,

\[
\tau_F \equiv \frac{D}{u_F^2} \left[ -1 + \sqrt{1 + \left(\frac{u_F}{\sqrt{D n_0}}\right)^2} \right] \quad .
\]  

(17)

The production (annihilation) rate of thermal \(K^+\overline{K}\) pairs per length unit is thus given by the universal function\(^8\)

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

(18)

where \(F_c = kT n_0 / 2\pi\). 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:
Diffusive limit: $F \ll F_c$ in (18) implies $\Gamma_D \equiv 4 D n_0^3$, and, explicitly

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

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

Ballistic limit: $F \gg F_c$ in (18) justifies the approximation $\Gamma_B \equiv 2 u_F n_0^2$, i.e.

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

The two results in (15) and (20) differ by an interaction induced renormalization of the damping coefficient $\alpha$ in (15), $\alpha \to \alpha_{BL} = \alpha(m/\pi) (2/F\beta E_F)^{1/2}$. 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 $(F/m^2) < kT/E_0$, $\lambda_0^2$ is a small negative eigenvalue which, in addition to the Goldstone mode, can be treated as an approximate, collective variable to be integrated over.

References