Analytical determination of the production rate of thermal sine-Gordon solitons

Fabio Marchesoni*
Institut für Theoretische Physik, Rheinisch-Westfälische Technische Hochschule Aachen, D-5100 Aachen, Federal Republic of Germany
(Received 12 June 1986)

The equilibrium production rate of kink-antikink pairs in sine-Gordon systems subject to local thermal fluctuations is determined analytically. In the limit of strong damping the energy needed to nucleate a kink-antikink pair turns out to be three times the rest energy of a single kink. This result is interpreted in terms of a three-body mechanism of pair production.

The problem of the escape of a Brownian particle out of a one-dimensional metastable potential well has been treated by means of a variety of techniques.[1] The extension of some of such techniques to deal with metastable minima of multidimensional systems is also well established.[2,3] A rather different situation is described by the perturbed sine-Gordon (SG) equation

$$\phi_{tt} - c_0^2\phi_{xx} + \omega_0^2 \sin\phi = -\alpha\phi_t + \zeta(x,t) \;, \tag{1}$$

where α is the damping constant and $\zeta(x,t)$ is a thermal random force with $\langle\zeta\rangle = 0$ and correlation function[4]

$$\langle \zeta(x,t)\zeta(x',t')\rangle = 2\alpha k_B T\,\delta(t-t')\delta(x-x') \;. \tag{2}$$

In the discrete representation of Eq. (1), $\zeta(x,t)$ corresponds to an array of Gaussian (in time) δ-correlated random forces acting on each site independently and with equal intensities. Analogously, Eq. (1) describes an ensemble of Brownian particles bound by a multistable periodic potential and interacting (linearly) with their nearest neighbors.

The related problem of the escape of (a set of) these particles over a potential barrier in the presence of thermal fluctuation cannot be treated as a straightforward application of the stochastic analysis of Refs. 2 and 3. Difficulties arise because of the discrete "translational" invariance $\phi \to \phi + 2\pi$ of the system [Eqs. (1) and (2)]. In the absence of an external bias[4] we cannot identify a saddle point in the energy surface through which the field (or chain) configuration is to pass. A saddle-point configuration should be a stationary solution of the unperturbed SG equation such that its energy increases or remains constant *in all but one* direction as one moves away from it. This difficulty has been underestimated in Ref. 5 where the details of the activating mechanism are purposely neglected.

In this Brief Report we present an alternative determination of the *equilibrium* production rate of thermal kinks. As a major distinction between geometrical and thermal kinks we recall that the latter ones are always produced in pairs.[4] The relevance of the process of solitonic pair production in many fields of condensed matter physics and electronics has been well elucidated by several authors (see Refs. 4 and 5, and references therein).

In the Büttiker-Landauer theory of nucleation, kinks and antikinks are immediately driven apart due to the presence of an external constant force. An unperturbed doublet (kink+antikink) configuration, whose distance between the kink and antikink depends on the intensity of the external bias, plays the role of a saddle-point configuration. However, when the external field is switched off, the doublet configuration energy is neutral under variation of the distance between its components. The situation is even more complicated when we admit the presence of other pairs which can influence to some extent the motion of the newly formed pair and act on it as a time-dependent external field of force.[6]

Since a detailed study of such a mechanism is far too complex, we propose an equilibrium statistical mechanical treatment. According to the authors of Refs. 7 and 8 we assume that any solution of the SG equation can be described as a dilute gas of unperturbed kinks and antikinks. This picture has been proved to work quite well in the limit of low temperature.[8] The spatial size of the kinks is negligible compared to their mean free path, and their collisions can be treated as elastic. Under such approximations the mean kink (antikink) density per unit of length is given by

$$\langle n\rangle = \left(\frac{2}{\pi}\right)^{1/2} \frac{\omega_0}{c_0} (\beta E_0)^{1/2} e^{-\beta E_0} \;, \tag{3}$$

where $\beta = 1/k_B T$ and $E_0 = 8\omega_0 c_0$ is the rest energy of a single kink (antikink).

The continuum limit of the Fokker-Planck equation corresponding to the discretized system [Eqs. (1) and (2)] coincides with the classical partition function of the Hamiltonian system from which the unperturbed SG equation derives.[9] This implies that the canonical ensemble description of Refs. 7 and 8 also can be easily extended to determine the statistical properties of the solutions of the SG equation in the presence of local thermal fluctuations. In particular, the perturbed SG solutions still can be depicted as a dilute gas of kinks and antikinks with mean density $\langle n\rangle$, as in Eq. (3).

The presence of a fluctuation term $\zeta(x,t)$, however, modifies two important properties of such a gas, namely, the interaction mechanism and the "free" movement of its components. Kink-(anti)kink collisions can be analyzed by extending the perturbation technique of McLaughlin and Scott.[9,10] The collision of two unperturbed kinks is elastic and the effective potential acting between them is repulsive.[6] Under the action of a frictional term this bouncing mechanism is likely to remain almost unchanged. The situation is markedly distinct in the case of

 ©1986 The American Physical Society

kink-antikink collisions. Kink and antikink attract each other and, in the absence of thermal fluctuation, their interaction is reflectionless. The interaction, on the contrary, becomes *destructive*[11] unless the friction losses are not compensated by the energy input of a suitable external field of force.

At low temperatures any solution to the SG equation departs from the representation as a linear combination of kinks and antikinks only when the distance between two components is about twice the kink size. Between two successive collisions each kink (antikink) travels with constant velocity if $\alpha=\zeta=0$ or undergoes a process of translational diffusion in the presence of thermal fluctuations. In both cases the individual mean energy is given by $k_BT/2$.[8,9]

We recently proposed a new description[9] of the diffusional process of a single kink (antikink) subject to the stochastic perturbation of Eq. (1). Our approach consisted in generalizing the perturbation technique of Ref. 10 to deal with fluctuating (both in space and in time) fields of force. We proved that at the first order in the perturbation parameter α [$\alpha \ll \omega_0$ and T fixed and small, i.e., $\beta E_0 \ll 1$ (Ref. 10)] the effect of the thermal fluctuation amounts to activating a Brownian movement of the kink structure which, in turn, is not distorted. The random motion of the perturbed kink is described by a Langevin equation (LE)

$$\dot{p} = -\alpha p + \sqrt{E_0}\gamma(t) \ . \tag{4}$$

Here p denotes the kink momentum

$$p(t) = E_0 u(t)/[1-u^2(t)]^{1/2} \ ,$$

$u(t)$ the kink velocity, and $\gamma(t)$ a random stochastic fluctuation in time with correlation functions

$$\langle\gamma\rangle = 0, \ \langle\gamma(t)\gamma(t')\rangle = 2\alpha k_B T\delta(t-t') \ . \tag{5}$$

The physical scenario leading to our determination of the pair production rate is now clear. A doublet configuration annihilates each time a destructive collision between kink and antikink occurs. At equilibrium the frequency of such phenomenon must coincide with the rate of production of an equivalent pair. We assume that at equilibrium only $n_\gamma(\alpha)$ pairs out of $\langle n\rangle$ survive interaction in the presence of stochastic fluctuation $\gamma(t)$. This means that the thermal energy of a certain fraction $\eta(\alpha) = [\langle n\rangle - \langle n_\gamma(\alpha)\rangle]/\langle n\rangle$ of colliding kinks and antikinks is high enough for them to pass through each other.

We start calculating the time a kink needs to encounter destructively an antikink. The mean distance L between annihilating kink and antikink is given by $(\langle n\rangle - \langle n_\gamma\rangle)^{-1}$. The equilibrium quadratic displacement of the kink center of mass can be determined from the LE(4) (Ref. 12) in the limit of low temperatures, i.e., $p(t) = E_0 u(t)$,

$$\langle \Delta x^2(t)\rangle = qt/\alpha^2 - q(1-e^{-\alpha t})/\alpha^3 \ , \tag{6}$$

where $q = 2\alpha/\beta$. In the overdamped regime, i.e., for $\alpha t \gg 1$, we approximate

$$\langle \Delta x^2(t)\rangle \simeq qt/\alpha^2 \ . \tag{7}$$

Equating $\langle \Delta x^2(t)\rangle$ with L^2 gives the kink mean diffusion time before a destructive collision, i.e., the lifetime τ of a thermal kink (or antikink). We note that at low temperatures τ is fairly large so that limit (7) can be realized at values of α for which LE(4) is still reliable ($\alpha \ll \omega_0$).[9]

The mean pair production rate for unit of length μ is then defined as $2\langle n\rangle/\tau$. Employing Eqs. (3) and (8) we obtain our prediction in the overdamped limit

$$\frac{\mu_0}{\eta(\infty)} = 4\frac{\omega_0^2}{\alpha}\left(\frac{8}{\pi}\right)^{3/2}\left(\frac{\omega_0}{c_0}\right)^2 (\beta E_0)^{1/2} e^{-3\beta E_0} \ . \tag{8}$$

(i) Prediction (8) is quite surprising. In the limit of strong damping, kinks and antikinks colliding annihilate,[10] i.e., $\eta(\infty)=1$. The Arrhenius factor appearing in μ_0 implies that the total energy needed to nucleate a kink-antikink pair is three times the rest energy of a single kink and not twice the kink energy as one might naively expect.[5] Actually, what the result suggests is that a kink-antikink creation in the limit of strong damping can only occur in the presence of a spectator. As an intuitive argument, we would interpret such a spectator as a *thermalized* kink (or antikink) attracting the antikink (or kink) partner of the newly nucleating doublet, thus exerting a pressure which contributes to expand the nucleating doublet to infinity.

(ii) The Büttiker-Landauer theory for nucleation of overdamped soliton motion[4] must also be quoted here. As a starting point in their analysis these authors assume that nucleation of kink-antikink doublets is triggered by an external field of force F. The activation energy $2E_0(F)$ ($\leq 2E_0$) in the Arrhenius factor thus obtained depends on F. Since the activation energy cannot change abruptly from $2E_0(F)$ to $3E_0$, we advocate the existence of a crossover field F_c which separates the two different mechanisms. Such a crossover would occur when the external force due to the field of force $2\pi F_c$ equals the opposite attraction k_BT/l exerted on the doublet components by thermal motion of the spectator. l denotes here the distance moved by thermalized solitons before destructive interaction. It follows that $2\pi F_c \simeq k_BT\langle n\rangle$. In this limit, however, the Büttiker and Landauer approach does not apply.[4]

In this Brief Report we have calculated the equilibrium pair production rate for a SG system at low temperature. The main features of our predictions are likely to be relevant to the modeling of chemical reactions in condensed phase as well.[13,14] A many-body activation mechanism could be invoked, indeed, to explain experimental observations which do not match the classic Kramers model.[14] This discussion will be reported in further publications.

I wish to thank the Alexander von Humboldt Stiftung for financial aid and Professor B. U. Felderhof for hospitality at the Institut für Theoretische Physik (RWTH-Aachen). Professor L. Váquez, Professor N. G. van Kampen, and Dr. W. Renz are thanked for useful discussions and the Fondazione A Della Riccia for financial support.

*Permanent address: Dipartimento di Fisica, Università di Perugia, I-06100 Perugia, Italy.

[1]For a recent review, see T. Fonseca, J. A. N. F. Gomes, P. Grigolini, and F. Marchesoni, Adv. Chem. Phys. **62**, 389 (1985).
[2]J. S. Langer, Ann. Phys. (N.Y.) **54**, 258 (1969); **41**, 108 (1967).
[3]R. Landauer and J. A. Swanson, Phys. Rev. **121**, 1668 (1961).
[4]M. Büttiker and R. Landauer, Phys. Rev. A **23**, 1397 (1981).
[5]W. Wonneberger, Physica A **103**, 543 (1980).
[6]J. Rubinstein, J. Math. Phys. **11**, 258 (1970).
[7]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B **11**, 3535 (1975).
[8]J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **22**, 477 (1980).
[9]F. Marchesoni, Phys. Lett. **115A**, 29 (1986).
[10]D. W. McLaughlin and A. C. Scott, Phys. Rev. A **18**, 1652 (1978).
[11]We remark that breather configurations (whose energy is smaller than or equal to E_0) play no role in the statistical mechanical picture of Refs. 7 and 8. Further results about this question will be presented elsewhere.
[12]H. Risken, *The Fokker-Planck Equation,* Springer Series in Synergetics, Vol. 18 (Springer-Verlag, Berlin, 1983), Chap. 6.
[13]H. A. Kramers, Physica **7**, 284 (1940); M. Büttiker, H. P. Harris, and R. Landauer, Phys. Rev. B **28**, 1268 (1983); F. Marchesoni, *ibid.* **32**, 1827 (1985); W. Renz and F. Marchesoni, Phys. Lett. **112A**, 124 (1985).
[14]F. Marchesoni, Chem. Phys. Lett. **110**, 20 (1984); Adv. Chem. Phys. **63**, 389 (1985), and references therein.