

Exact kink-gas phenomenology of deformable systems at low temperatures

David Yemélé¹ and Timoléon C. Kofané^{1,2}

¹Laboratoire de Mécanique, Faculté des Sciences, Université de Yaoundé I, BP 812 Yaoundé, Cameroun
²Laboratoire de Physique de l'Université de Bourgogne, Avenue Alain Savary, BP 400, 21011 Dijon, France

(Received 30 December 1999; revised manuscript received 30 March 2000)

The low-temperature thermodynamics of a class of one-dimensional nonlinear deformable Klein-Gordon systems is studied by means of a simple soliton-gas picture. The lowest order correction to the free energy due to the interaction between solitons is obtained. The result is in complete agreement with that of the transfer integral method.

The role played by the soliton (kink and antikink) excitations in the thermodynamics of one-dimensional nonlinear systems was discussed for the first time by Krumhansl and Schrieffer (KS).¹ By using a phenomenological calculation (in which each soliton is treated as a particle in an "ideal gas" of solitons), they showed that the tunnel splitting between wells in the ϕ^4 potential is due to the solitons.¹ The work of Currie, Krumhansl, Bishop, and Trullinger (CKBT) (Ref. 2) has subsequently confirmed the transfer-integral method discussed by Scalapino, Sears, and Ferrell³ and proved by KS as exact if the influence of kinks on the phonon density of states is explicitly taken into account.

The analysis of CKBT was extended in two principal directions: (i) DeLeonardis and Trullinger⁴ have extended this phenomenology to a general class of the nonlinear rigid Klein-Gordon systems. More precisely, they have shown that explicit knowledge of phase-shift functions and internal mode frequencies is not needed to put forward the exactness of the ideal soliton-gas phenomenology at low-temperature, and a general formula for the soliton free energy was obtained. (ii) Another important aspect which has been considered by Sasaki,^{5,6} Tsuzuki and Sasaki⁷ is the effect of soliton-soliton interactions on statistical mechanics. A general formula for the second virial coefficient in the soliton free energy was derived.

However, these results concerning the sine-Gordon (SG) and other rigid potentials are very encouraging, but they remain nevertheless limited in their applicability to real physical systems. Since, in those systems, the shape of the nonlinear one-site potential may deviate considerably from that attributed to the local potential.^{8,11} For example, in hydrogen-bonded system, the large displacement of heavy ions can significantly modify the barrier height of the double-well potential associated with the light protons.¹² Also, in the adsorption systems, the shape of the substrate potential deviates from the SG potential.¹³ Hence the use of the deformable systems in the present work is dictated by our effort to go beyond the mathematical problem and obtain results that may be useful for real materials that undergo structural changes such as shape distortion, variations of crystalline structures or conformational changes, in some regions of their physical parameters. Such materials cannot be satisfactorily described by substrate potentials with constant parameters, for which much work has been already done in

the context of their thermodynamical behavior. As a consequence the general formula derived by DeLeonardis and Trullinger⁴ and Sasaki⁶ for the free energy fails and may be improved. It is then of interest to study this phenomenology for more general deformable systems.

Our aim in the present work is to derive, in the classical limit, a general formula for the soliton contribution and for the second virial coefficient in the free energy for a class of deformable nonlinear Klein-Gordon family within the soliton-gas phenomenology. The general soliton density formula proposed by DeLeonardis and Trullinger⁴ for all rigid potentials such as ϕ^4 , double quadratic (DQ), SG, double sine-Gordon (DSG), etc., is corrected and extended to deformable models where soliton-soliton contribution is obtained via a soliton gas picture by Sasaki.⁶ The exactness of the low-temperature phenomenology is demonstrated for the deformable sine-Gordon system¹⁰ (as an example) where the soliton contribution to the free energy could be found and compared to the transfer-integral result.¹⁴

The general class of one-dimensional nonlinear Klein-Gordon systems in the notation of CKBT is defined by the Hamiltonian

$$H = A \int_{-\infty}^{\infty} dx \left[\frac{1}{2} \left(\frac{\partial \theta}{\partial t} \right)^2 + \frac{1}{2} C_0^2 \left(\frac{\partial \theta}{\partial x} \right)^2 + \omega_0^2 V(\theta) \right], \quad (1)$$

where $\theta(x, t)$ is the dimensionless field, C_0 and ω_0 are characteristic velocity and frequency, respectively. The ratio $d_0 = C_0/\omega_0$ determines the characteristics length scale for variation in θ while the constant A sets the energy scale. $V(\theta)$ is the dimensionless local potential which is assumed to have at least two degenerate absolute minima at $\theta = \theta_1$ and $\theta = \theta_2$ with $\theta_1 < \theta_2$, separated by a barrier about the point θ_{12} . For periodic potential, θ_1 and θ_2 denote any two adjacent absolute minima in $V(\theta)$.

In the case of the periodic deformable sine-Gordon potential of Remoissenet and Peyrard defined by^{10,14}

$$V(\theta) = \frac{(1-r)^2}{2} \frac{1 - \cos \theta}{1 + r^2 + 2r \cos \theta}, \quad |r| < 1 \quad (2)$$

we have $\theta_1 = 0$, $\theta_2 = 2\pi$, and $\theta_{12} = \pi$. The curvature at minima are

$$V''(\theta_1) = V''(\theta_2) = \begin{cases} \alpha^2 & \text{for } r < 0, \\ 1/\alpha^2 & \text{for } r > 0, \end{cases} \quad (3)$$

where $\alpha = (1 - |r|)/(1 + |r|)$. The prime indicates the derivatives with respect to θ . The shape of the potential is defined by the parameter r . For $r > 0$ the potential (2) has flat bottoms separated by thin barriers, while for $r < 0$, it has the shape of sharp wells separated by flat wide barriers. When $r = 0$, this potential reduces to a sinusoidal SG potential. Hereafter, we refer to the potential (2) as the Remoissenet-Peyrard (RP) potential.

The nonsinusoidal RP potential has been used to calculate the pinning energy of kinks due to the discreteness of substrate lattices,^{13,15} as a model for reconstructive surface growth,¹⁶ and to describe the complicated exchange-mediated diffusion mechanism.¹⁷ It has been also used to calculate the diffusion coefficient of adsorbates in metallic substrates,¹⁸ the nucleation rate of kink-antikink pairs at low temperatures and in the limit of strong damping.¹⁹ Finally, the deformable spin hamiltonian has been recently introduced²⁰ and two classes of topological soliton have been calculated in the model of long-range interatomic interactions with RP potential.²¹ Periodic and chaotic behaviors in several models of driven nonlinear oscillators have been discussed in great detail.^{22,23} However little is known about thermodynamical behavior in the RP potential. Only the work by the present authors where the free energy at low temperatures has been calculated exactly by means of the transfer-integral method.¹⁴ The use of the deformable RP potential is finally dictated by the fact that the exactness between this integral-operator result and the exact kink-gas phenomenology result outlined here may be viewed as a prove of this phenomenology.

We shall have the occasion to use the following improved temperature-independent numerical constants constructed from the potential^{4,6,7}

$$\zeta = \int_{\theta_1}^{\theta_2} d\theta [2V(\theta)]^{1/2}, \quad (4)$$

$$\eta = \int_{\theta_{12}}^{\theta_2} d\theta \left[\frac{[V''(\theta_2)]^{1/2}}{[2V(\theta)]^{1/2}} - \frac{1}{\theta_2 - \theta_1} \right], \quad (5)$$

$$v = \frac{1}{8} (\theta_1 - \theta_2)^2 \zeta^{-1} \exp(2\eta). \quad (6)$$

The parameter ζ follows from the calculation of the soliton rest energy while η results from the calculation of the soliton contribution in the free energy. Note the change in the definition of the parameter η , which in the case of deformable systems, has been renormalized by the factor $V''(\theta_2)^{1/2}$. Also, the last parameter v depends on ζ and η , and follows from the phase shift associated with kink-phonon interaction which of course depends on the particular potential at hand. This phase shift contains all of the information concerning kink-phonon interaction that one need to construct the phenomenological free-energy density of soliton. All the three parameters are essentials in the derivation of this soliton free-energy without knowledge of the soliton wave form and its small oscillations.

For the deformable sine-Gordon potential defined by Eq. (2), we have

$$\zeta^{(1)} = (1 - \alpha^2)^{-1/2} \tan^{-1}[(1 - \alpha^2)^{1/2}/\alpha],$$

$$\eta^{(1)} = \ln\left(\frac{4\alpha}{\pi}\right) + \frac{(1 - \alpha^2)^{1/2}}{\alpha} \tan^{-1}[(1 - \alpha^2)^{1/2}] \quad (7a)$$

and

$$\zeta^{(2)} = \alpha(1 - \alpha^2)^{-1/2} \tanh^{-1}[(1 - \alpha^2)^{1/2}],$$

$$\eta^{(2)} = \ln\left(\frac{4}{\pi\alpha}\right) + (1 - \alpha^2)^{1/2} \tanh^{-1}[(1 - \alpha^2)^{1/2}], \quad (7b)$$

where the upper scripts (1) and (2) stand for the case $r < 0$ and $r > 0$, respectively. Hence, from Eqs. (7), the quantity v takes the following value:

$$v^{(1)} = \alpha(1 - \alpha^2)^{1/2} \exp\left\{2 \frac{(1 - \alpha^2)^{1/2}}{\alpha} \tan^{-1} \left[\frac{(1 - \alpha^2)^{1/2}}{\alpha} \right] \right\} / \tan^{-1}[(1 - \alpha^2)^{1/2}/\alpha], \quad (8a)$$

$$v^{(2)} = (1 - \alpha^2)^{1/2} \exp\{-2(1 - \alpha^2)^{1/2} \tanh^{-1} [(1 - \alpha^2)^{1/2}] / \alpha^2 \tanh^{-1} [(1 - \alpha^2)^{1/2}]\}. \quad (8b)$$

In the limit $r \rightarrow 0$, we recovered the sine-Gordon case:^{9,10} $\zeta = 1$, $\eta = \ln 4/\pi$, $v = 1$. For potentials with more than one type of barrier, there is a constant η , ζ and v of the form Eqs. (4)–(6) for each type.

The system described by the Hamiltonian (1) possesses stable small amplitude solutions (in the bottom of each potential well) with the dispersion relation

$$\omega_k^2 = \omega_r^2 + C_0^2 k^2, \quad \omega_r^2 = \omega_0^2 V''(\theta_2), \quad (9)$$

where ω_r is a frequency of oscillations of an isolated particle at the bottom θ_2 of the substrate potential and to the wave vector. In the continuum soliton limit, the system admits soliton solutions (kink and antikink) of velocity $\mu < C_0$ (Ref. 10) with energy

$$E_k = C_0 \omega_0 A \zeta \gamma \quad (10)$$

and with pseudokink width

$$d_s = d_0 / V''(\theta_2)^{1/2}, \quad (11)$$

where $\gamma = (1 - \mu^2/C_0^2)^{1/2}$, and ζ defined by Eq. (4). The static kink energy is then given by

$$E_s = M_s C_0^2, \quad M_s = A \omega_0 \zeta / C_0, \quad (12)$$

where M_s is the kink rest mass

From a phenomenological point of view, CKBT showed that the low-temperature free-energy density of an ideal gas of slowly moving kinks (and antikinks) has the form²

$$f_s^{id} = -k_B T n_s^{id}, \quad (13)$$

where n_s^{id} is the total density of soliton kinks plus antikinks while k_B is the Boltzmann constant and T the temperature. Here, the density of solitons are so small that the interaction between solitons can be neglected in the first approximation. By making use of the collective coordination of the ideal-gas approximation, n_s^{id} is given by the relation

$$n_s^{id} = C \int \frac{dp}{2\pi\hbar} e^{-\beta\Delta E(p)} \quad (14)$$

where

$$\Delta E(p) = M_s C_0^2 + \frac{p^2}{2M_s} + \Sigma_k \quad (15)$$

represents the difference between the free energies in the presence and absence of a soliton with momentum P , in the nonrelativistic limit ($\mu \ll C_0$). The last term of Eq. (15) is the self-free energy (see Ref. 2) of a static soliton, which represents the change in phonon free energy due to the interaction with soliton. It can be obtained without detailed knowledge of the kink wave form or the small oscillation about the kink:

$$\Sigma_k = -k_B T \ln(v^{1/2} \beta \hbar \omega_r) \quad (16)$$

where $\beta = 1/k_B T$, and v is the constant defined in Eq. (6), while ω_r , is given by Eq. (9). In Eq. (16) the characteristic frequency of the system has been replaced by the renormalized frequency ω_r [see Eq. (9)]. The constant C in Eq. (14) is the model-dependent numerical constant.^{6,7} $C = 1$ for systems with double-well potentials such as the ϕ^4 , the parametrized double-well potentials,^{8,9} and $C = 2$ for systems with periodic potentials such as the sine-Gordon, the deformable sine-Gordon defined in Eq. (2). Substitution of Eqs. (15) and (16) into Eq. (14) and integration of Eq. (14) yields a general formula for low-temperature density of solitons (kinks plus antikinks) of a given type

$$n_s^{id} = \frac{2C}{d_s} \left(\frac{\beta E_s}{2\pi} \right)^{1/2} v^{1/2} e^{-\beta E_s}. \quad (17)$$

By substituting Eq. (16) into Eq. (13), we obtain the free-energy density

$$f_s^{id} = -\frac{2C}{\beta d_s} \left(\frac{\beta E_s}{2\pi} \right)^{1/2} v^{1/2} e^{-\beta E_s}. \quad (18)$$

Substituting Eqs. (8) and (12) into Eqs. (17) and (18), one finds that Eqs. (17) agree with the transfer-integral result for the deformable sine-Gordon potentials [see Eq. (3.21) of Ref. 14]. Note also that, in Eqs. (17) and (18), the characteristic length scale of the system d_0 has been replaced by the renormalized length scale d_s which is the pseudokink width.

We now come to the interaction between solitons. For this aim, let us consider a classical gas of solitons (kink and antikink) with mass M_s and energy E_s . The potential energy or the two solitons interaction energy evaluated by calculating energy of periodic solutions (soliton lattices) is given in a general form by

$$U(x) = \sigma_1 \sigma_2 E_s v e^{-|x|/d_s}, \quad (19)$$

for $|x| \gg d_s$, where x is the distance between the two interacting solitons, σ_1 and σ_2 are the polarities of these solitons labeled by 1 and 2, and v the numerical constant defined in Eq. (6). The spatial shift in the trajectory of particles caused by an elastic collision can be easily evaluated:⁷

$$\Delta(p_1 - p_2) = 2d_s \ln(2v^{1/2} M_s C_0 / |p_1 - p_2|), \quad (20)$$

in the limit $p_1, p_2 \ll M_s C_0$, where p_1 and p_2 are the asymptotic momenta of the two solitons which is a constant of motion. The position shifts Δ is responsible for the change in the momentum space due to the interaction.⁶ In the thermodynamics of a soliton gas, it may be interpreted as an effective size of the soliton in collision. Hence, the average size of solitons is then given by

$$B = \int dp_1 dp_2 \Delta(p_1 - p_2) p(p_1) p(p_2) = d_s \ln(4\Gamma v \beta E_s), \quad (21)$$

where $\Gamma = 1,7810, \dots$, is the Euler constant, and

$$P(p_i) = \left(\frac{2\pi M_s}{\beta} \right)^{1/2} \exp\left(-\frac{\beta p_i^2}{2M_s} \right), \quad i = 1, 2 \quad (22)$$

is the momentum distribution of probability of solitons in the ideal-gas approximation. The quantity B designates the second virial coefficient in the free energy. Consequently, the free energy density f_{sc} and the total density of solitons are

$$f_{sc} = -k_B T n_s^{id} (1 - B n_s^{id}), \quad n_{sc} = n_s^{id} (1 - 2B n_s^{id}), \quad (23)$$

in the second virial approximation. Substitution of v by his expression (8) for the deformable sine-Gordon potential into Eqs. (17) and (21) yields the transfer-integral result [see Eqs. (3.19) and (3.20) of Ref. 14].

The second virial coefficient B is the logarithmic temperature dependence which is attributed to the exponential decay of the interaction potential between solitons at large distances. To evaluate it, we have assumed elastic collisions between solitons. This is true only in the integrable systems, similar to SG systems. However numerical integrations of the equation of motion in the nonintegrable systems show that, solitons dissipated part of their energies into small oscillations or phonons. For some initial conditions soliton and antisoliton annihilate in pair leaving small oscillations only. Thus, the result obtained here suggests that the effect of emission and absorption of phonons by solitons does not appears in the second virial term. It could be probably appears in higher order term in the virial development of the free energy, as pointed out by Sasaki.⁶

From Eq. (23) it appears that, all the quantities entering in these formulas (E_s , d_s , v , and η) can be obtained directly from the particular one-site deformable potential, as demonstrated by DeLeonardis and Trullinger⁴ in the case of the rigid potential. This has the practical consequence that at low temperature, explicit knowledge of the kink wave form and its small oscillations (or internal modes) are not needed and the free energy of a particular deformable potential could be found easily by means of a simple integrals over the potential.

To conclude this report, note that phenomenological calculations for very low-temperature soliton statistical mechanics have reached a stage such that they agree with the analytic transfer-integral results. However, the phenomenological approach has still restricted to the rigid potentials or scaled potentials. For this purpose, we have extended the

soliton-gas theory, which gives accurate values for the scaled potential such as ϕ^4 sine-Gordon, to both the deformable ϕ^4 and deformable sine-Gordon potentials. This generalization may be viewed as a first step toward the thermodynamics of the quantum deformable systems which is now in progress.

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