Statistical mechanics of a nonlinear deformable sine-Gordon model

David Yemélé and Timoléon C. Kofané
Laboratoire de Mécanique, Faculté des Sciences, Université de Yaoundé I, B.P. 812, Yaoundé, Cameroun
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The low-temperature thermodynamic properties of a deformable sine-Gordon model are studied by means of the transfer-integral method. Using asymptotic methods from the theory of differential equations depending on a large parameter, the lowest-order corrections due to the interactions between solitons as well as the first-order lattice corrections to the free energy are evaluated. They are strongly dependent on the deformable parameter r. It appears that the entropy of the system is an increasing function of r. A physical interpretation of the result shows that, in the system, disorder increases as r varies from 0 to 1 and decreases when r varies from 0 to -1. [S0163-1829(97)01926-7]

I. INTRODUCTION

In the last few decades, a great amount of attention has been devoted to the low-temperature statistical mechanics of one-dimensional (1D) nonlinear models of condensed matter systems which support kinklike or solitary wave solutions of the associated field equation of motion. This attention has been motivated by the important role played by the kink in many areas of condensed matter physics: dislocations in crystals,[1–3] planar domains walls in ferromagnets[4] and ferroelectrics,[5–7] propagating flux quanta in Josephson transmission lines,[8] nonlinear spin waves,[9] incommensurate systems,[10,11] and bond-alternation domain walls in polyacetylene[12,13] to name only a few. It has been shown, through the transfer integral operator (TIO) method or ideal-gas phenomenology, that the low-temperature thermodynamics of the systems are sensitive to and even dominated by solitons.[5,14–16] Their presence in the system is signaled by the term E_s in the Arrhenius factor in the low-temperature free energy, where E_s is the static soliton energy. This picture has proved to work quite well in the continuum limit (strong coupling between adjacent particles) where the soliton width has to be large enough to avoid the discreteness effects of the lattice.

In some materials, the soliton width is just a few lattice spacings and the discreteness effects cannot be neglected.[17] Their influence on the properties of nonlinear systems supporting kinklike solutions was investigated by several authors.[18–28] Those studies have carried out a large variety of effects, namely, the modification of kink velocity and energy, and the pinning of the kink center of mass between lattice sites. Recently, the influence of the lattice discreteness on the thermodynamic properties has received a little attention.[26,29–32] Trullinger and Sasaki[30] have examined the entirely separate question of the effects of discreteness on the results of the TIO method. They obtained the lowest-order discreteness corrections to the pseudo-Schrödinger equation approximation to the transfer integral equation for the entire class of kink-bearing Hamiltonians. Also, the effect of soliton-soliton interactions on statistical mechanics has been considered only recently[33–35] and its study as well as that of the discreteness effects has still been restricted to the sine-Gordon (SG) and ϕ^4 systems, the only exception to our knowledge being the recent work by Dikandé and Kofané[26] on the deformable ϕ^4 systems.

In spite of the fact that the results concerning the SG model as well as the ϕ^4 and other rigid models are very encouraging, they remain nevertheless limited in their applicability to real physical systems, since it is unlikely that physical condensed matter systems will be ''exactly'' described by either of the special cases of these potentials with defined shapes. For example, it is established that under variation of some physical parameters such as the temperature and pressure, some physical systems may undergo changes which are either shape distortions, variations of crystalline structures, or conformational changes. Also, in the hydrogen-bonded system, the large displacement of the heavy ions can significantly modify the barrier height of the double-well potential associated with the light proton.[36] It appears then relevant to look for a wider class of potentials useful to describe nonlinear excitations in real materials and model field theories. Thus a few deformable models have appeared in the literature such as parametrized double-well potentials.[36–40] Also, deformable SG models have been proposed.[41–43] The dynamic and thermodynamic properties as well as the chaotic behavior[44–46] of some of these deformable nonlinear systems have been studied.

In this paper, we investigated the low-temperature classical mechanics of a 1D atomic chain with a deformable periodic potential whose shape can be varied continuously as a function of the parameter r and which has the SG shape as a particular case.[41] The lowest-order discreteness effects as well as the soliton-soliton interactions will be taken into account in our study. The paper is organized as follows: In Sec. II, we briefly present the deformable lattice, while Sec. III is devoted to the low-temperature classical mechanics of the model. In this section, the Schrödinger-like equation resulting from the TIO method is solved in the limit of low temperatures by means of the procedure outlined in Ref. 29 based on the asymptotic methods from the theory of differential equations depending on large parameter.[47] Next, we evaluated the thermodynamic functions, and in Sec. IV, we summarize our results.

II. MODEL DESCRIPTION

The system we wish to consider is a chain of particles of mass m harmonically coupled, separated from each other in

the x direction with lattice spacing a and placed in the field of a nonlinear substrate potential $V(\phi,r)$. The Hamiltonian of this discrete chain [in the notation of Currie, Krumhansl, Bishop, and Trullinjer[16] (CKBT)] may be written as

$$H=\sum_i Aa\left\{\frac{1}{2}\,\dot{\phi}_i^2+\frac{C_0^2}{2a^2}\,(\phi_{i+1}-\phi_i)^2+\omega_0^2V(\phi_i,r)\right\}, \tag{2.1}$$

where ϕ_i is the scalar dimensionless longitudinal displacement of the ith particle on a 1D lattice. The constant $A\sim ma$ sets the energy scale of the system, and C_0 and ω_0 are a characteristic velocity and frequency, respectively. Here the overdot denotes time differentiation. The nonlinear ''one-site potential'' to which we concentrate our attention is that introduced by Remoissenet and Peyrard (RP),[41]

$$V(\phi,r)=(1-r)^2\,\frac{1-\cos\phi}{1+r^2+2r\,\cos\phi}, \tag{2.2}$$

where $|r|<1$. As this parameter varies, the amplitude of the potential remains constant with degenerate minima $2\pi n$ and maxima $(2n+1)\pi$, while its shape changes. At $r=0$, the RP potential model reduces to the well-known SG potential.

The system described by the Hamiltonian (2.1) possesses stable small-amplitude solutions (in the bottom of the potential well $\phi=2\pi n$) with the dispersion relation

$$\omega_g^2=\omega_r^2+(4C_0^2/a^2)\sin^2(ga/2),\quad \omega_r=\frac{1-r}{1+r}\,\omega_0, \tag{2.3}$$

where ω_r is a frequency of oscillations of an isolated particle at the bottom of the substrate potential and g the wave vector. With the help of the expression of ω_r and using the measured values of ω_0, it is more reliable to determine the parameter r directly from experimental data. An estimate for, e.g., an H/W adsystem (hydrogen atoms adsorbed on a tungsten surface) yields $r\simeq -0.3$.[48] Apart from the small-amplitude solutions, in the case of strong coupling between adjacent particles ($d=C_0/\omega_0\gg a$) the system admits two families of implicit kink solutions with velocity v given in term of the moving coordinates $s=(1-v^2/C_0^2)^{-1/2}(x-vt)$ by[41,42]

$$\frac{s}{d^{(1)}}=\mathrm{sgn}(\phi-\pi)\left\{\frac{(1-\alpha^2)^{1/2}}{\alpha}\,\tan^{-1}\left[\frac{(1-\alpha^2)^{1/2}}{[\alpha^2+\tan^2(\phi/2)]^{1/2}}\right]+\tanh^{-1}\frac{\alpha}{[\alpha^2+\tan^2(\phi/2)]^{1/2}}\right\}, \tag{2.4a}$$

with the rest energy

$$E_s^{(1)}=8AC_0\omega_0(1-\alpha^2)^{-1/2}\tan^{-1}[(1-\alpha^2)^{1/2}/\alpha], \tag{2.4b}$$

for $-1<r\leqslant 0$ and

$$\frac{s}{d^{(2)}}=\mathrm{sgn}(\pi-\phi)\times\left\{(1-\alpha^2)^{1/2}\,\tanh^{-1}\left[\frac{(1-\alpha^2)^{1/2}}{[1+\alpha^2\tan^2(\phi/2)]^{1/2}}\right]-\tanh^{-1}\frac{1}{[1+\alpha^2\tan^2(\phi/2)]^{1/2}}\right\}, \tag{2.5a}$$

with the rest energy

$$E_s^{(2)}=8AC_0\omega_0\alpha(1-\alpha^2)^{-1/2}\tanh^{-1}[(1-\alpha^2)^{1/2}], \tag{2.5b}$$

for $0\leqslant r<1$, with

$$\alpha=\frac{1-|r|}{1+|r|},\quad d^{(1)}=d\alpha,\quad d^{(2)}=d/\alpha, \tag{2.6}$$

where $d^{(j)}$ $(j=1,2)$ are the ''pseudokink widths.'' For $r=0$, Eqs. (2.4) and (2.5) reduce to the usual SG kink. When r tends to 1, $d^{(2)}$ tends to infinity. On the other hand, when r decreases and tends to -1, $d^{(1)}$ tends to zero. Thus the kink extension is not only determined by the characteristic length scale d, but also by the curvature of the minima of the potential. It is important to note that when r tends to -1, even if the neighboring particles are sufficiently closed (strong coupling), the kink extension could be just a few lattice spacings and, consequently, the discreteness effects on soliton dynamics[42] and thermodynamic properties could not be neglected.

III. LOW-TEMPERATURE STATISTICAL MECHANICS

The classical canonical partition function for systems governed by the Hamiltonian (2.1) for distribution of the density of states in phase space is given in the factored form $Z=Z_\phi Z_\phi$ by making use of the TIO method[25] with[5]

$$Z_\phi=\left(\frac{2\pi Aa}{\beta h^2}\right)^{N/2},\quad Z_\phi=\sum_{n=0}^{\infty}\exp(-\beta AL\omega_0^2\varepsilon_n), \tag{3.1}$$

where $\beta=1/k_BT$, k_B being the Boltzmann constant, h the Planck constant, T the temperature, N the number of particles, and $L=Na$ the length of the chain. Here ε_n is the eigenvalue of a pseudo-Schrödinger equation

$$-\left(\frac{1}{2m^*}\right)\frac{d^2}{d\phi^2}\,\psi_n(\phi)+V_{\mathrm{eff}}(\phi,r)\psi_n(\phi)=\tilde{\varepsilon}_n\psi_n(\phi), \tag{3.2}$$

with

$$\tilde{\varepsilon}_n=\varepsilon_n-V_0,\quad V_0=(-1/\rho)\ln\left(\frac{2\pi a^2}{\rho d^2}\right)^{1/2},\quad \rho=Aa\beta\omega_0^2,$$

$$m^*=A^2\beta^2C_0^2\omega_0^2. \tag{3.3}$$

The temperature-dependent parameter m^* plays the role of an ''effective mass'' of a particle moving in the 1D effective potential[30]

$$V_{\rm eff}(\phi,r)=V(\phi,r)-\Lambda\left(\frac{dV(\phi,r)}{d\phi}\right)^2, \quad \Lambda=a^2/(24d^2). \tag{3.4}$$

In the thermodynamic limits ($L\to\infty$, $N\to\infty$, $L/N=$const), Z_ϕ is dominated by the lowest eigenvalue $\tilde{\varepsilon}_0$ and the free energy per unit length, $f=-(1/\beta L)\ln Z$, becomes

$$f=(-1/2\beta a)\ln\left(\frac{2\pi Aa}{\beta h^2}\right)+A\omega_0^2V_0+A\omega_0^2\tilde{\varepsilon}_0. \tag{3.5}$$

It is apparent that, to evaluate f, the main problem we are faced with consists in the investigation of the lowest eigenvalue $\tilde{\varepsilon}_0$ of the Schrödinger operator. We first concentrate our attention on the continuum limit ($\Lambda=0$). In the low-temperature regime ($\beta\ll 1$), there are several ways to find the approximate eigenvalue $\tilde{\varepsilon}_0$, namely, the improved WKB methods. In the following we use the procedure outlined in Ref. 29 which has the advantage of making a clear distinction between various contributions to the free energy: phonons, solitons, soliton-solitons, etc. Following this procedure, the calculation of the ground state $\tilde{\varepsilon}_0$ is similar to the one performed by Croitoru *et al.*[29,44] for the asymptotical evaluation of the eigenspectrum for the SG potential case. It yields

$$\tilde{\varepsilon}_0^{(j)}=\tilde{\varepsilon}_{00}^{(j)}(1+4\nu_{\rm inf}). \tag{3.6}$$

The superscripts (1) and (2) stand for the case $-1<r\leqslant 0$ and $0\leqslant r<1$, respectively. From now we shall use this notation. Here $\tilde{\varepsilon}_{00}^{(j)}$ is the first term in the asymptotic expansion of the lowest eigenvalue of the isolated potential well given by

$$\tilde{\varepsilon}_{00}^{(1)}=\frac{1}{2\alpha\sqrt{m^*}}, \quad \tilde{\varepsilon}_{00}^{(2)}=\frac{\alpha}{2\sqrt{m^*}}. \tag{3.7}$$

It can be readily obtained by solving Eq. (3.2) with an approximated form of the potential $V(\phi,r)$ by a second-order Taylor expansion about $\phi=0$ (lowest-order harmonic oscillator level). This approximation is accurated if the temperature is sufficiently low.

The quantity $\nu_{\rm inf}$ is the small parameter related to the small shifts from the eigenvalue of an isolated well due to the presence of the other degenerate minima of the potential $V(\phi,r)$. The presence of these degenerate minima leads to the tunnel splitting of the lowest level $\tilde{\varepsilon}_{00}^{(j)}$ of the isolated well into continuous bands. The lower extremity ($\nu_{\rm inf}$) can be found using the boundary conditions for the wave function of Eq. (3.2) and its derivative. As previously mentioned,[32] the tunneling terms ($\nu_{\rm inf}$) are directly related to the soliton contribution to the free energy. It follows that

$$-\nu_{\rm inf}=\nu, \tag{3.8}$$

where ν verifies the equation[32]

$$\exp[-2\lambda I-2\nu(1+\ln 2)+(1/2)(1+4\nu)\ln(1+4\nu)-1/2] = \frac{-2\sqrt{\pi}}{\Gamma(-\nu)}\frac{\Gamma(\nu+1/2)}{\Gamma(1/2)}\exp(-i\pi\nu). \tag{3.9}$$

The constant I is related to the potential $V(\phi,r)$ through

$$I=\int_{\tau_2}^{\pi}\sqrt{-q(\tau)}\,d\tau, \tag{3.10}$$

where τ_2 is the right turning point of the isolated well centered at $\phi=0$ given by

$$\tau_2^{(1)}\simeq\left(\frac{\alpha^2\tilde{\varepsilon}}{2-\tilde{\varepsilon}(1-\alpha^2)}\right)^{1/2}, \quad \tau_2^{(2)}\simeq\left(\frac{\tilde{\varepsilon}}{2\alpha^2+\tilde{\varepsilon}(1-\alpha^2)}\right)^{1/2}. \tag{3.11}$$

The integration of Eq. (3.10) yields[49]

$$I=2\sqrt{2}\left\{(1-\alpha^2)^{-1/2}\tan^{-1}[(1-\alpha^2)^{1/2}/\alpha]-\alpha(\tilde{\varepsilon}_0^{(1)2}/8) \times\left[\ln(32/\tilde{\varepsilon}_0^{(1)2})+1+2\frac{(1-\alpha^2)^{1/2}}{\alpha}\tan^{-1}[(1-\alpha^2)^{1/2}/\alpha]\right\}\right. \tag{3.12a}$$

for $-1<r\leqslant 0$ and

$$I=2\sqrt{2}\{\alpha(1-\alpha^2)^{-1/2}\tanh^{-1}[(1-\alpha^2)^{1/2}]-(\tilde{\varepsilon}_0^{(2)2}/8\alpha) \times[\ln(32/\tilde{\varepsilon}_0^{(2)2})+1-2(1-\alpha^2)^{1/2} \times\tanh^{-1}[(1-\alpha^2)^{1/2}]\} \tag{3.12b}$$

for $0\leqslant r<1$, where $\tilde{\varepsilon}_0^{(1)}$ and $\tilde{\varepsilon}_0^{(2)}$ are defined in Eq. (3.7).

To evaluate the various soliton contributions, a systematic method of evaluating ν as a serie expansion in $\theta=e^{-\beta E_s^{(j)}}\ll 1$ was given by Grecu and Visinescu.[32] Up to second order, ν is obtained as

$$\nu=\theta\nu_1+\theta^2\nu_2+\cdots, \tag{3.13}$$

with

$$\nu_1^{(j)}=(16\sqrt{m^*}\tilde{C}^{(j)}/\pi)^{1/2},$$

$$\nu_2^{(j)}=2\nu_1^{(j)2}(\ln(32\gamma\sqrt{m^*}\tilde{C}^{(j)})-i\pi/2), \tag{3.14}$$

which follows from the substitution of Eq. (3.13) into Eq. (3.9), where

$$\tilde{C}^{(1)}=\exp\{[2(1-\alpha^2)^{1/2}/\alpha]\tan^{-1}[(1-\alpha^2)^{1/2}/\alpha]\}\alpha, \tag{3.15a}$$

$$\tilde{C}^{(2)}=\exp\{-2(1-\alpha^2)^{1/2}\tanh^{-1}[(1-\alpha^2)^{1/2}]\}/\alpha, \tag{3.15b}$$

and $\gamma=1.7810\ldots$ is Euler's constant. Equation (3.14) shows that ν_2 is imaginary with an imaginary part satisfying the relation

$$\text{Im}\ \nu_2^{(j)}=\pi\nu_1^{(j)}. \tag{3.16}$$

For $r=0$, this relation reduces to that obtained by Grecu and Visinescu[32] when they analyzed the lattice corrections to the free energy of the SG models. We will show that this imaginary part may be of importance for understanding of the system's behavior. A physical interpretation is given below. In the following, we consider only the real part of ν_2. From Eqs. (3.6), (3.8), and (3.13), the lowest eigenvalues $\tilde{\varepsilon}_0$ of the Schrödinger eigenvalue equation can be as follows:

$$\tilde{\varepsilon}_0^{(j)}=\tilde{\varepsilon}_{00}^{(j)}-4(16\sqrt{m^*}\tilde{C}^{(j)}/\pi)^{1/2}\tilde{\varepsilon}_{00}^{(j)}e^{-\beta E_s^{(j)}} \times[1-2(16\sqrt{m^*}\tilde{C}^{(j)}/\pi)^{1/2}e^{-\beta E_s^{(j)}}\ln(32\gamma\sqrt{m^*}\tilde{C}^{(j)})]. \tag{3.17}$$

Since we are presently in possession of the relevant parameters interfering in the construction of the thermodynamic properties of the model, we shall first estimate the basic thermodynamic function (free energy density). This energy can be separated into two parts. The part

$$f_{\rm ph}^{(j)}=(1/\beta a)\ln\left(\frac{\beta\hbar C_0}{a}\right)+A\omega_0^2\tilde{\varepsilon}_{00}^{(j)} \tag{3.18}$$

is due to the classical harmonic phonons. The second part $f_{\rm tun}$ contains the kink rest energy $E_S^{(j)}$. It is well known since the basic works of Krumhansl and Schrieffer[5] and CKBT (Ref. 16) that this term is kink (antikink) contribution to free energy density. Owing to the fact that $f_{\rm tun}$ contains the relevant information about manifestations of solitons in thermodynamic processes, it is rewritten in the more suggestive form[35]

$$f_{\rm tun}^{(j)}=-K_BTn_0^{(j)}(1-B^{(j)}n_0^{(j)}). \tag{3.19}$$

Also, the total density of kinks and antikinks is given by

$$n_{k-k}^{{\rm tot}(j)}=n_0^{(j)}(1-2B^{(j)}n_0^{(j)}), \tag{3.20}$$

with

$$n_0^{(j)}=\frac{2}{d^{(j)}}\left(\frac{2}{\pi}\right)^{1/2}(8\sqrt{m^*}\tilde{C}^{(j)})^{1/2}e^{-\beta E_s^{(j)}}, \tag{3.21}$$

$$B^{(j)}=d^{(j)}\ln(32\gamma\sqrt{m^*}\tilde{C}^{(j)}), \tag{3.22}$$

where $d^{(j)}$ are the pseudokink width defined in Eq. (2.6) and $n_0^{(j)}$ are the total density of kinks and antikinks within the ideal gas approximation. The coefficients $B^{(j)}$ are the logarithmic temperature dependence, which are attributed to the exponential decay of the interaction potential between soliton at large distances.[35] Equation (3.20) follows from the soliton-gas interpretation of the soliton free energy density according to the treatment of Ref. 35.

As we have evaluated the free energy density f, all other thermodynamic quantities can be readily obtained. The specific heat c_l per unit length is given by

$$c_l^{(j)}/K_B=\{(1/a)+n_0^{(j)}[(\beta E_s^{(j)}-1/2)^2-1/2]\}-n_0^{(j)2}d^{(j)} \times\{1-4\beta E_s^{(j)}[1-(B^{(j)}/d^{(j)})(\beta E_s^{(j)}-1)\}. \tag{3.23}$$

Similarly, the entropy s per unit length is given by

$$s^{(j)}/K_B=\left\{\frac{1}{a}[1-\ln(\beta\hbar C_0/a)-a/2d^{(j)}] +n_0^{(j)}(\beta E_s^{(j)}+1/2)\right\} +n_0^{(j)2}d^{(j)}(1-2\beta E_s^{(j)}B^{(j)}/d^{(j)}). \tag{3.24}$$

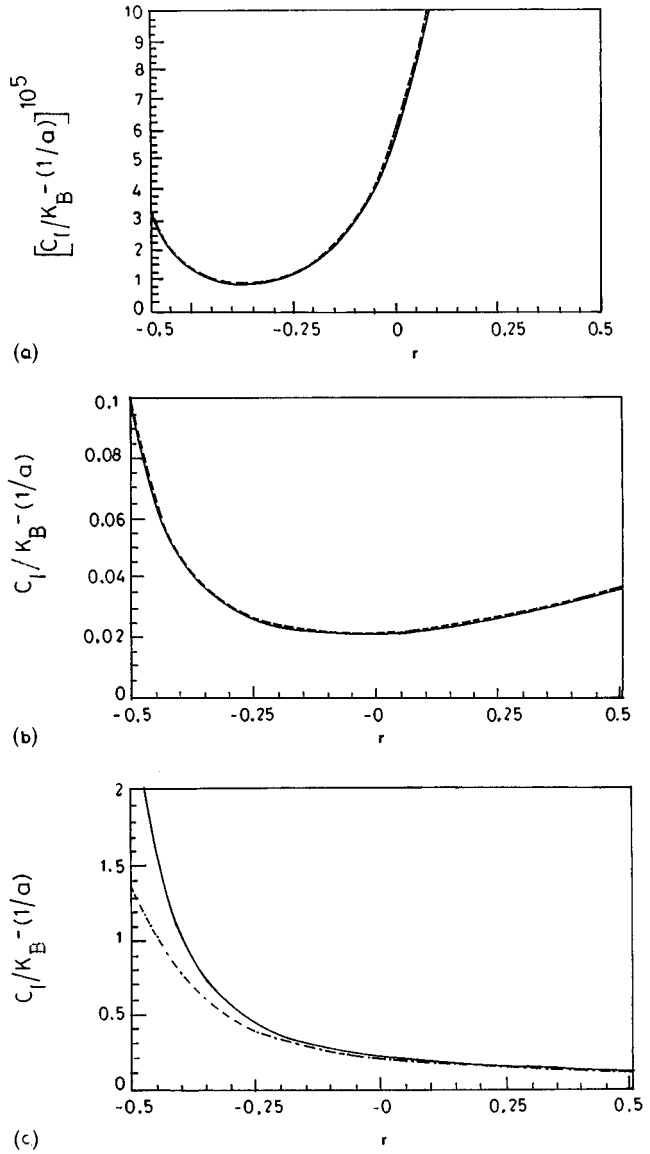

FIG. 1. Plot of the specific heat per unit length (in arbitrary units) vs r and for a few normalized temperature ($d=10a$) $T^*=K_BT/(8A\omega_0C_0)$, $a=1$: (a) for $T^*=0.05$, (b) for $T^*=0.1$, and (c) for $T^*=0.15$. The dotted curves are the results of Eqs. (3.23), while the solid lines are the results of the term containing in the first bracket only (i.e., without the correction term due to soliton-soliton interactions).

Equations (3.23) and (3.24) give the low-temperature thermodynamic properties of the deformable SG system. The terms proportional to $n^{(j)2}$ designate the corrections due to soliton-soliton interactions. As one can readily see from the numerical analysis of the above formulas of thermodynamic functions as well as the total kink density, all these quantities are reduced by the correction terms whatever the value of the deformable parameter r. These correction terms decrease when the temperature decreases and become negligible for very small temperature (see, for example, Fig. 1 for the specific heat). Also, the analysis of c_1 as a function of r shows that the contribution of the correction term decreases when r increases and becomes negligible when $r>0$ (Fig. 1). Consequently, the contribution of soliton-soliton interactions is useful particularly for $r<0$.

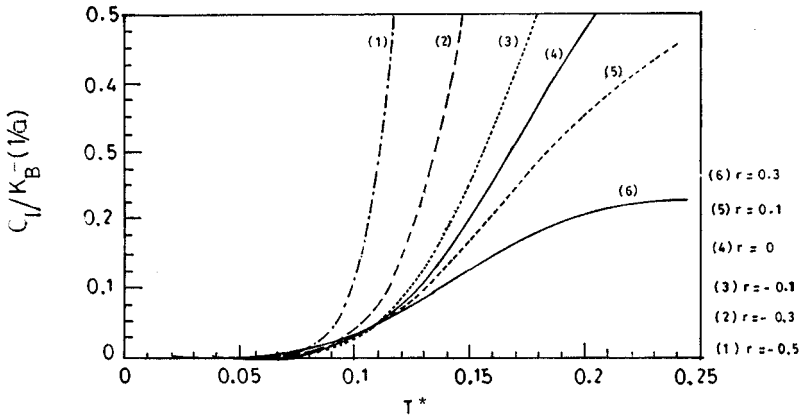

FIG. 2. Specific heat as a function of $T^* = K_B T/(8A\omega_0 C_0)$, for a given r. See the increasing value of c_l with T^*.

The analysis for a given temperature of these thermodynamic quantities as a function of r shows that their variations pass into a minimum at r_0, which depends on the temperature. As r increases from -1 to r_0, these quantities decrease to a minimum and increase with r from r_0 to 1 (Fig. 1). r_0 is different from a function to other one. Otherwise, the entropy s is an increasing function of r. This increasing behavior of the entropy can be understood if we appeal to the fact that an increase of the deformable parameter r leads to an increase of the kink width. Consequently, the entropy of the system increases. It is also seen, as can be expected, that these thermodynamic properties increase with temperature (for example, see Fig. 2 for the case of the specific heat).

Let us look at the lattice corrections to the free energy density. As pointed out by Trullinger and Sasaki,[30] the first lattice corrections are taken into account if the potential $V(\phi,r)$ is replaced by an effective potential $V_{\rm eff}(\phi,r)$ defined in Eq. (3.4). Using the same procedure of the preceding paragraph, the free energy density is given (available for small r) by

$$f^{(j)} = f^{(j)}_{\rm ph} + f^{(j)}_{\rm tun}, \tag{3.25a}$$

where

$$f^{(j)}_{\rm ph} = (1/\beta a)\ln\left(\frac{\beta\hbar C_0}{a}\right) + \frac{1}{2\beta d^{(j)}}\,[1 - a^2/(24 d^{(j)2})], \tag{3.25b}$$

$$f^{(j)}_{\rm tun} = \frac{2}{d^{(j)}}\left(\frac{2}{\pi}\right)^{1/2}(8\sqrt{m^*})^{1/2}(1 - a^2/(48 d^{(j)2}))e^{-\beta E^{(j)}_{sc}} \times\left\{1 - 2\left(\frac{2}{\pi}\right)^{1/2}(8\sqrt{m^*})^{1/2}e^{-\beta E^{(j)}_{sc}}\ln(32\gamma\sqrt{m^*})\right\}, \tag{3.25c}$$

with

$$E^{(1)}_{sc} = E^{(1)}_s(1 - \Lambda/3\alpha^2), \quad E^{(2)}_{sc} = E^{(2)}_s(1 - \Lambda\alpha^2/3), \tag{3.26}$$

where Λ is defined in Eq. (3.4).

The term $f_{\rm tun}$ designates the contribution of kinks and antikinks to the free energy, while $f_{\rm ph}$ is due to classical harmonic phonons. It is important to note that $f_{\rm ph}$ is easily identified with the first terms in the series expansion in powers of (a^2/d^2) of the exact free energy of a phonon gas,

$$f_{\rm ph} = (1/2\pi\beta)\int_{-\pi/a}^{+\pi/a} dg\ \ln(\beta\hbar\omega_g) \tag{3.27}$$

(with $\hbar = h/2\pi$), where ω_g is given by Eq. (2.3).

The preceding formulas of the free energy density show us that the correction terms involving (a^2/d^2) are proportional to the curvature of the potential $V(\phi,r)$ at its minima. This result is in agreement with the expectation of Ref. 30. In the model under consideration, this curvature is $1/\alpha^2$ for $r \leqslant 0$ and α^2 for $r \geqslant 0$. As one can readily see, these correction terms are very small for the model with $r \geqslant 0$ indeed, even for a/d as large as unity. However, it appears that these terms are appreciable when r approaches -1.

The Arrhenius factor appearing in $f_{\rm tun}$ $(E^{(j)}_{sc})$ implies that the rest energy of the soliton is corrected by the factor $(1 - \Lambda/3\alpha^2)$ (for $r \leqslant 0$) and $(1 - \Lambda\alpha^2/3)$ (for $r \geqslant 0$) by the lattice discreteness effects. This energy is therefore lowered below the continuum zero-order value $E^{(j)}_s$. Such lowering has also been obtained recently by other authors.[27,30–32] The discreteness correction appearing in Eq. (3.26) for the kink rest energy can be interpreted as a downward renormalization of the kink creation energy.[30,50]

Before concluding this work, we wish to make a few comments about the imaginary part of the tunneling contribution of the ground-state energy (ν_2). Note that a similar relation has been obtained by Zinn-Justin[51] in model field theories. Later this result has been extended in condensed matter physics by Grecu and Visinescu,[32] and our result represents a generalization for a nonlinear deformable sine-Gordon model. In fact, particular interest[51,52] has been, some years ago, devoted to find the large order behavior of perturbation theory in the case of potentials with degenerate minima in which a divergent result was found in quantum mechanics for the ground-state energy. To avoid this inconsistency where the instanton does not correspond to a periodic path, Zinn-Justin[51] has performed a large-order estimate for the perturbative expansion of the ground-state energy around an instanton–anti-instanton path configuration leading to an imaginary part contribution. For an analytical potential possessing degenerate minima, such as ϕ^4 field theory, the kink (instanton) configuration has topological charge $+1$, while the antikink (anti-instanton) has topological charge -1. Both configurations communicate between the adjacent wells of the potential. However, the kink-antikink configuration (resulting from inelastic scattering of

kinks) corresponds in a configuration from vacuum to vacuum with topological charge (determined from the boundary conditions at plus and minus infinity) zero.

Beside the above comment, one can add the following general observation: The problem we are faced up deal with the soliton-soliton stability which is related to the complete integrability of the corresponding wave equation. In such a case, when the solitary waves interact, they are always scattered elastically, preserving asymptotically their shape. The integrability also permits an analytical study of the multisoliton interactions such as in the sine-Gordon model. In many real physical systems, the basic models are not integrable such as the ϕ^4 model. Many numerical studies of the collisions of solitary waves in nonintegrable systems have been done (see Ref. 53 and references therein). From the soliton-gas theory[35,50] to integrable or nonintegrable systems, one can say that the real part of Eq. (3.13) results from the elastic scattering of solitons. However, solitons lose or gain energy in the form of radiation during their collisions (inelastic scatterings). The consequence is that the final velocity of the soliton is less than its initial velocity. Also, these inelastic scatterings can lead to a chaotic behavior of the system.[45] Sometimes, creation and annihilation of the soliton-antisoliton pairs occurs, and are accompanied by absorptions and emissions of phonons. Therefore it is possible that the imaginary part of ν_2 may be related to the inelastic scattering contribution of solitons or to the so-called vacuum sector of solutions with topological charge zero. In this case, following Langer,[54] it is now interpreted in the same way as the imaginary component of a resonance energy in quantum-field theory, namely, as a quantity describing the finite lifetime of each state of the periodic potential.

IV. SUMMARY

This work intended to investigate the low-temperature thermodynamic properties of the 1D deformable sine-Gordon model by means of the TIO method. Explicit expressions of the specific heat and entropy as well as total kink density have been obtained. For a given temperature, all these functions vary and pass into a minimum when r increases, except the entropy which increases for increasing r. Such behavior of the entropy is understandable if we appeal to the fact that the increase of the deformable parameter r leads to the increase of the wide spread of disorder in the system.

Owing to the fact that the model is not a completely integrable one and to the importance of the discreteness effects in many physical applications involving nonlinear solitonlike excitations, the lattice corrections and soliton-soliton contributions to the free energy have been calculated. All these results reduce to that of the SG system in the limit $r=0$.[30,32] The main conclusion which derives from the above result is that the lattice correction as well as the soliton-soliton contributions to the thermodynamic properties at low temperature is more relevant for physical systems with a negative value of the deformable parameter r and negligible for those with a positive value of r. This result is not surprising since the increase of the kink width (increase of r) leads to the decrease of the soliton-soliton interactions and the lattice discreteness effects.

In spite of the interesting results obtained in this paper, much remains to be done. For example, there may exist materials for which it is not possible to assume the small parameter r as we have done when deriving the lattice corrections to the free energy.

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