Low-temperature statistical mechanics of kink-bearing systems with a Remoissenet-Peyrard substrate potential: Influence of anharmonic interactions

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The low-temperature statistical mechanics of one-dimensional nonlinear Klein-Gordon with anharmonic interparticle interaction subject to the Remoissenet-Peyrard substrate potential is studied by means of the transfer integral method. We show that the quantitative effects of the anharmonicity of the interparticle pair potential to the thermodynamic properties of the system are controlled by temperature. They are negligible for very low temperatures and become more and more important as the temperature increases. Furthermore, the first lattice corrections to the thermodynamic quantities are temperature dependent and are sensitive to the deformability of the system.

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I. INTRODUCTION

Many physical properties of real systems are directly related to nonlinear effects produced by anharmonic interactions. These systems which usually support the propagation of localized nonlinear excitations have been intensively examined in connection with nonthermalization process, nonlinear transport of energy in atomic and molecular chains.[1] The model which describes the interactions between particles of the system by an empirical potential has the advantage that the dynamical behavior and the thermodynamic properties of the system can be studied. In other words, analytical studies and numerical experiments can be conducted which simulate the essential of the physical phenomena exhibited by the system. The basic model is nonlinear Klein-Gordon (NKG) model where the particles may be considered as coupled to nearest neighbors via an harmonic interaction potential and subjected to a nonlinear on-site or substrate potential. If the substrate potential has degenerate minima [double-well shape like ϕ^4 and deformable ϕ^4 (Refs. 2 and 3) or periodic degenerate minima like sine-Gordon (sG) and deformable sG potential (Refs. 2 and 4)], solitary waves can exist and can be calculated exactly in the continuum limit. In addition, soliton-soliton interactions and the interactions between solitons and other elementary excitations such as phonons can also be calculated. The result being of particular importance when investigating, within the soliton gas approach, the statistical mechanics of the system in order to determine the thermal density of thermally activated kink excitations and their contribution in the thermodynamic quantities of the system.[5–7] The inclusion of interactions between low-lying excitations (kink and phonons) allows to obtain precise agreement between this phenomenology and the exact result of the transfer integral operator (TIO) method.[2,5–7]

The basic NKG model takes into account only the harmonic approximation of the nearest-neighbor interaction potential. However, in real systems interaction between particles is more complicated and can be consequently modeled by an anharmonic function. There is also a clear evidence that kink internal modes are not only limited to the case of an harmonic interparticle interaction since it was found that such solutions occur also in anharmonic interparticle interaction.[8,9] Note that the inclusion of anharmonic interactions is dictated by some experimental investigations. For example, some previous models have indicated that the inclusion of anharmonic forces can give an answer to the problem of heat conduction in one-dimensional insulating solids.[10] It is the merit of Rosenau and Hyman,[11] who investigated a special type of Korteweg-de Vries equation to discover that solitary waves may become compact in the presence of nonlinear dispersion. Such solitary waves, which are characterized by the absence of infinite tail, have been called compactons. Since this pioneering work, the kink compacton excitations have become the subject of many works. To cite just a few examples, we mention that Dusuel *et al.*[12] have demonstrated that kink compacton can also appear in the NKG systems with anharmonic interaction pair potential. Recently, it has been demonstrated that, localized breathing mode with an "almost compact support" (stationary breather compacton),[13] drop compactons, cups, peak solitons, and defects[14] can appear in the generalized NKG model with ϕ^4 substrate potential. The ability of a compacton like kink to execute a stable ballistic propagation in this discrete Klein-Gordon system[15] has been also investigated. Note also the study of lattice effects on the motion of kink compactons[16] which has revealed that the effects of lattice discreteness and the presence of a linear coupling between sites are detrimental to a stable ballistic propagation of compactons, and that of the exact calculation of the poly-kink compactons in the generalized NKG model with deformable periodic symmetric and asymmetric double well potentials of Peyrard and Remoissenet.[17]

Since condensed matter physics is one of the areas of the physics where the dynamical behavior of the systems can be satisfactorily described by the generalized NKG model and where the number of low-lying excitations is thermally controlled, the study of the statistical mechanics of this model is therefore an interesting problem. In this spirit, we have studied recently the low-temperature statistical mechanics of the

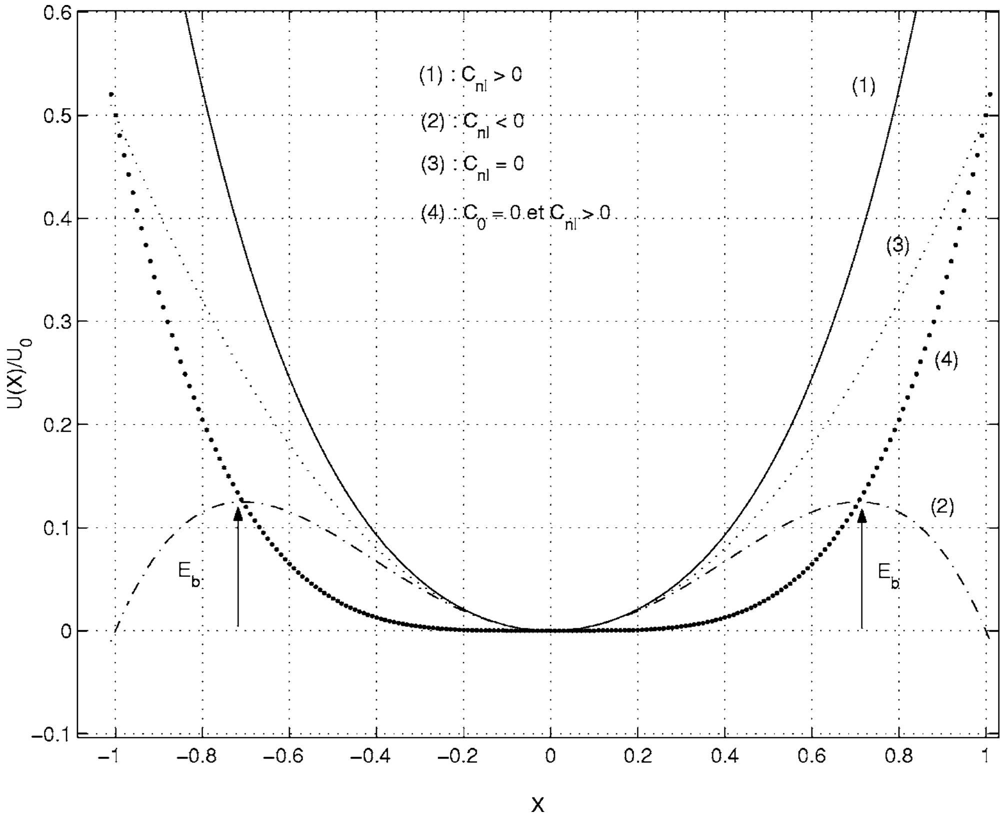

FIG. 1. Interaction pair potential of the nearest-neighbor particles $U(X)/U_0$ defined by Eq. (2.2), as a function of the reduced relative displacement between particles $X=(\phi_{i+1}-\phi_i)/X_0$ where $U_0=2C_0^4/|C_{nl}|$ in unit of Aa, and $X_0=C_0 a\sqrt{2/|C_{nl}|}$. It is important to distinguish two quite different situations according to the sign of the NICC C_{nl}, (i) $C_{nl}>0$, in this case; X_0 may be viewed as the relative displacement for which the contribution of the two terms in the IPP are identical and are equal to $U_0/2$. Accordingly, for $X<1$, the IPP is dominated by the harmonic term while the opposite situation occurs when $X>1$. (ii) $C_{nl}<0$, here, X_0 is a critical displacement since for this displacement, the IPP is zero and may become negative if $(\phi_{i+1}-\phi_i)>X_0$, that is, $X>1$. The IPP is nonconvex and presents a barrier at $X=\pm\sqrt{2}/2$ with height $U_1=C_0^4/4|C_{nl}|=U_0/8$.

generalized NKG systems with rigid substrate potentials such as the sG and the ϕ^4.[18] We have shown that the presence of kink compactons in the thermodynamic properties of the system is signaled by terms proportional to $\exp[-\chi(\beta E_{kc})^{3/4}]$ in the low-temperature free-energy, where E_{kc} is the static kink compacton energy and χ a temperature independent coefficient. In addition, by means of the TIO method, we have shown that the first lattice corrections to these thermodynamic quantities are temperature dependent.[19] In the present work, we focus our attention on the influence of anharmonic interparticle interaction on the thermodynamic quantities of this model which is extended to include the deformability of the substrate potential. Here, we restrict our analysis to the case where the system exhibits the kink solitons.

The organization of the paper is as follows. In Sec. II we present the model under consideration. In the limit of strong coupling between adjacent particles, the equation governing wave propagation in the lattice is derived and the qualitative behavior of the system is analyzed. In Sec. III, by means of the TIO method associated with the asymptotic methods from the theory of differential equations depending on a large parameter,[20] we derive the thermodynamic quantities of the system exhibiting the kink solitons. The influence of lattice effects to the free energy of the system is also considered. Finally, a brief summary and concluding remarks are done in Sec. IV.

II. MODEL AND KINKLIKE EXCITATIONS

The system under consideration consists of N particles of mass m placed on a one-dimensional lattice of lattice spacing a, oriented in the direction of the a axis. The Hamiltonian of this discrete chain may be written as follows:

$$H = Aa\sum_i \left[\frac{1}{2}\left(\frac{d\phi_i}{dt}\right)^2 + U(\phi_{i+1}-\phi_i) + \omega_0^2 V_{\mathrm{RP}}(\phi_i)\right], \quad (2.1)$$

where

$$U(\phi_{i+1}-\phi_i) = \frac{C_0^2}{2a^2}(\phi_{i+1}-\phi_i)^2 + \frac{C_{nl}}{4a^4}(\phi_{i+1}-\phi_i)^4, \quad (2.2)$$

is the interaction potential of the nearest-neighbor particles or interparticle pair potential (IPP) represented in Fig. 1 with ϕ_i the dimensionless displacement of the *ith* particle and

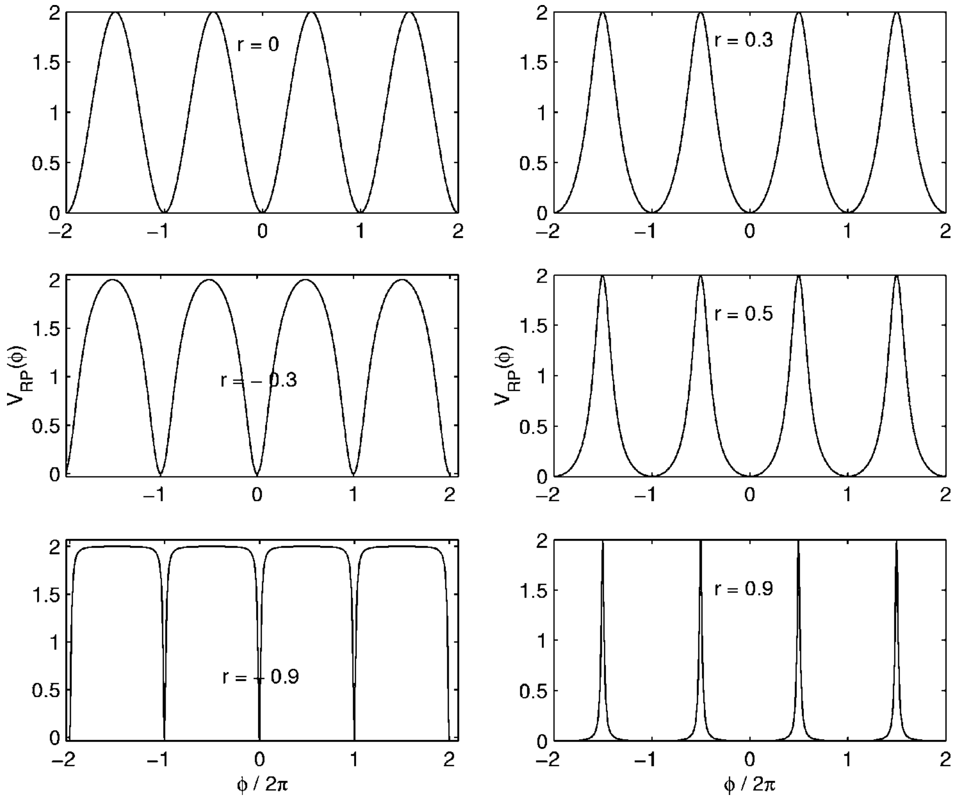

FIG. 2. Substrate potential $V_{RP}(\phi)$ for different values of the shape parameter r.

where C_{nl} determines the anharmonicity of this IPP. The constant $A \approx ma$ sets the energy scale of the system. The last term of Eq. (2.1) is the external potential or substrate potential. Here we focus our attention on the periodic deformable potential introduced by Remoissenet and Peyrard (RP)[4]

$$V_{\mathrm{RP}}(\phi_i) = (1-r)^2 \frac{1-\cos\phi_i}{1+r^2+2r\cos\phi_i}, \tag{2.3}$$

where the parameter $r(|r|<1)$ determines the shape. As r varies, the amplitude of the substrate potential remains constant with degenerate minima $2\pi n$ and maxima $(2n+1)\pi$, while its shape changes (see Fig. 2). This shape is controlled by the curvatures of the potential at the minima, that is $V''_{\mathrm{RP}}(2\pi n)=\alpha^2$ for $r>0$ and $V''_{\mathrm{RP}}(2\pi n)=1/\alpha^2$ for $r<0$, and at the maxima $V''_{\mathrm{RP}}[(2n+1)n]=-1/\alpha^2$ for $r>0$ and $V''_{\mathrm{RP}}[(2n+1)n]=-\alpha^2$ for $r<0$, where the parameter α is related to r through the following relation:

$$\alpha = \frac{1-|r|}{1+|r|}. \tag{2.4}$$

At $r=0$, that is $\alpha=1$, the RP potential reduces to the well-known sG potential. In addition, when the nonlinear interparticle coupling coefficient (NICC) $C_{nl}=0$, the model described by the Hamiltonian (2.1) reduces to the basic Hamiltonian previously used by CKBT (Ref. 2) and describing the basic NKG systems.

Two different regimes can occur according to whether the characteristic lengths of the system

$$d_0 = C_0/\omega_0 \quad \text{and/or} \quad \gamma_0 = (3|C_{nl}|/4\omega_0^2)^{1/4}, \tag{2.5}$$

are on the order of the lattice constant a or large compared to a. The first situation results when the interaction energy between neighbors is small compared to the on-site potential. In this case we are faced with the discrete system. In the opposite situation where the linear and nonlinear couplings between sites are strong enough ($d_0 \gg a$ and $\gamma_0 \gg a$) to ensure that the variation of ϕ_i from site to site are quite small, one can use the standard continuum approximation $\phi_i(t) \to \phi(x,t)$ and expand $\phi_{i\pm 1}$ with $x=ia$. Under these conditions, the Hamiltonian (2.1) is transformed approximately to

$$H = A \int dx \left[\frac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2 + \frac{C_0^2}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{C_{nl}}{4}\left(\frac{\partial\phi}{\partial x}\right)^4 + \omega_0^2 V_{\mathrm{RP}}(\phi) \right]. \tag{2.6}$$

In the following, we shall have occasion to use both forms, (2.1) and (2.6), of the Hamiltonian of the system. The discrete form (2.1) is used in obtaining exact statistical mechanical results via the TIO method, whereupon the explicit process of taking the continuum limit follows. The continuum form (2.6) is used to study the nature of excitations of the system; these excitations arise as solutions to the

Euler-Lagrange equation of motion of particles of the system following from Eq. (2.6):

$$\frac{\partial^2\phi}{\partial t^2} - \left[C_0^2 + 3C_{nl}\left(\frac{\partial\phi}{\partial x}\right)^2\right]\frac{\partial^2\phi}{\partial x^2} + \omega_0^2\frac{dV_{\rm RP}(\phi)}{d\phi} = 0. \tag{2.7}$$

We look for travelling waves of the form $\phi(x,t)=\phi(s)=\phi(x-\nu t)$ where s is a single independent variable depending on ν which is an arbitrary velocity of propagation. Thus, Eq. (2.7) is transformed to

$$\frac{d^2\phi}{ds^2}\left[1 + 3\zeta\gamma_L^2\left(\frac{d\phi}{ds}\right)^2\right] - \lambda\gamma_L^2\frac{dV_{\rm RP}(\phi)}{d\phi} = 0, \tag{2.8}$$

with the first integral given by

$$\left(\frac{d\phi}{ds}\right)^4 + \frac{2}{3\zeta\gamma_L^2}\left(\frac{d\phi}{ds}\right)^2 - \frac{4\lambda}{3\xi}[V_{\rm RP}(\phi) + C_1] = 0, \tag{2.9}$$

where $\zeta=C_{nl}/C_0^2$ is the reduced NICC, $\lambda=1/d_0^2$ is the effective depth of the substrate potential, $\gamma_L=(1-\nu^2/C_0^2)^{-1/2}$ the Lorentz factor and C_1 is a constant of integration.

When $C_{nl}=0$, Eq. (2.8) reduces to the standard continuous "RP model," that is the basic NKG system with the RP substrate potential, which admits solitary waves (kinks and breathers)[4] and linear waves solutions (phonons). These two kinds of excitations are well evidenced by the phase plane plot of the system. Similarly, the excitations of the system governed by Eq. (2.8) can be well analyzed by means of the phase plane plot. In order to obtain this phase plane, Eq. (2.8) is transformed into an equivalent autonomous equation

$$\frac{d\phi}{ds} = p,$$

$$\frac{dp}{d\phi} = \frac{\lambda\gamma_L^2}{p(1+3\gamma_L^2\zeta p^2)}\frac{dV_{\rm RP}(\phi)}{d\phi}. \tag{2.10}$$

In the low-velocity regime (nonrelativistic case), two situations occur according to whether the NICC C_{nl} is positive or negative.

(i) When $C_{nl}\geqslant 0$, the dynamical behavior of the system is qualitatively similar to that of the standard RP model. In fact, the phase plane plot exhibits, in one period of the substrate potential, three equilibrium points, and three kinds of phase trajectories [see for example Fig. 3(c)], the closed trajectories around the equilibrium point $(\phi,p)=(\pi,0)$ indicating the existence of linear and nonlinear phonons in the system, the open trajectories and finally the trajectories connecting the two other equilibrium points $(0,0)$ and $(2\pi,0)$ known as the separatrix which evidenced the existence of kinklike excitations in the system. These kinks are usually known as kink solitons. However, in the particular case where $\nu=C_0$, it has been demonstrated that these kinks may become compacts and are called kink compactons. Then the static kink compacton may be obtained only if $C_0=0$. In this latter case, the system is purely anharmonic.

(ii) When $C_{nl}<0$, the dynamical behavior of the system, materialized by the phase plane plot, changes qualitatively as a function of the strength of the NICC. Indeed, beside the classical points previously obtained, few more singular points appear. The exact position of these special points are derived from the singularity arising in the denominator of Eq. (2.10). Thus, we have $(\phi,p)=(0,\pm p_0)$, $(\pi,\pm p_0)$ and $(2\pi,\pm p_0)$ with $p_0=1/\gamma_L\sqrt{-3\zeta}$. For weak nonlinear interparticle coupling, in addition to the trajectories present in the standard RP model, one notes the appearance of two more families of open trajectories above and below the central region of Fig. 3(b) corresponding to new types of solutions which are not known in the standard RP model, confirming the fact that the anharmonicity in the IPP can allow the appearance of a rich variety of static and travelling excitations.[14] The separatrices are also present. However, when C_{nl} decreases upon reaching the threshold value

$$C_{nl} \geqslant C_{nl}^{th} \quad \text{with } C_{nl}^{th} = -\frac{C_0^4}{24\omega_0^2\gamma_L^4}, \tag{2.11}$$

the separatrices disappear on the phase plane plot [see Fig. 3(a)], indicating the breakdown of kink solitons like excitations. This disintegration of kink solitons has already been obtained for the rigid models such as the ϕ^4 and the sG (Ref. 18) as well as for the deformable double well models.[17]

Finally, the phase plane plot for the system governed by Eq. (2.8) with $r=-0.3$ shown in Fig. 4 demonstrates that the dynamical behavior of the system is qualitatively independent of the deformability parameter r of the system.

On the basis of the above results, it is now obvious that Eq. (2.8) admits different kinds of excitations among which are the kinks. These kinks are localized structure of permanent profile and verify the boundary conditions, $\phi\to\pm 0(2\pi)$ and $d\phi/ds\to 0$ when $s\to\pm\infty$, that is $C_1=0$ in the first integral equation (2.9). From this equation, it is easy to show that the shape of kink soliton is described by the following implicit relation:

$$\int_{\phi(s_0)=\pi}^{\phi(s)} \frac{d\phi}{2\sqrt{V_{\rm RP}(\phi)}}[1 + \sqrt{1+12\gamma_L^4\lambda\zeta V_{\rm RP}(\phi)}]^{1/2} = \pm\sqrt{\lambda}\gamma_L(s-s_0), \tag{2.12}$$

while its corresponding energy is given by

$$E_{ks} = 2AC_0\omega_0\gamma_L\int_0^{2\pi} d\phi\sqrt{V_{\rm RP}(\phi)} \times \frac{1+4\gamma_L^2\lambda\zeta V_{\rm RP}(\phi) + \sqrt{1+12\gamma_L^4\lambda\zeta V_{\rm RP}(\phi)}}{[1+\sqrt{1+12\gamma_L^4\lambda\zeta V_{\rm RP}(\phi)}]^{3/2}}. \tag{2.13}$$

The plus sign stands for the kink while the minus sign stands for the antikink. Due to the mathematical difficulties, we have not been able to integrate analytically Eqs. (2.12) and (2.13). Nevertheless, the numerical integration can be done. Figure 5 shows the profile of kink solitons for different values of the reduced NICC ζ and for few values of the deformability parameter r. It appears that, for a given value of r, the shape of the kink is sensitive to the anharmonicity of the IPP; its width increases with ζ. When $C_{nl}=0(\zeta=0)$, Eq. (2.8) reduces to the well-known standard equation without nonlinear

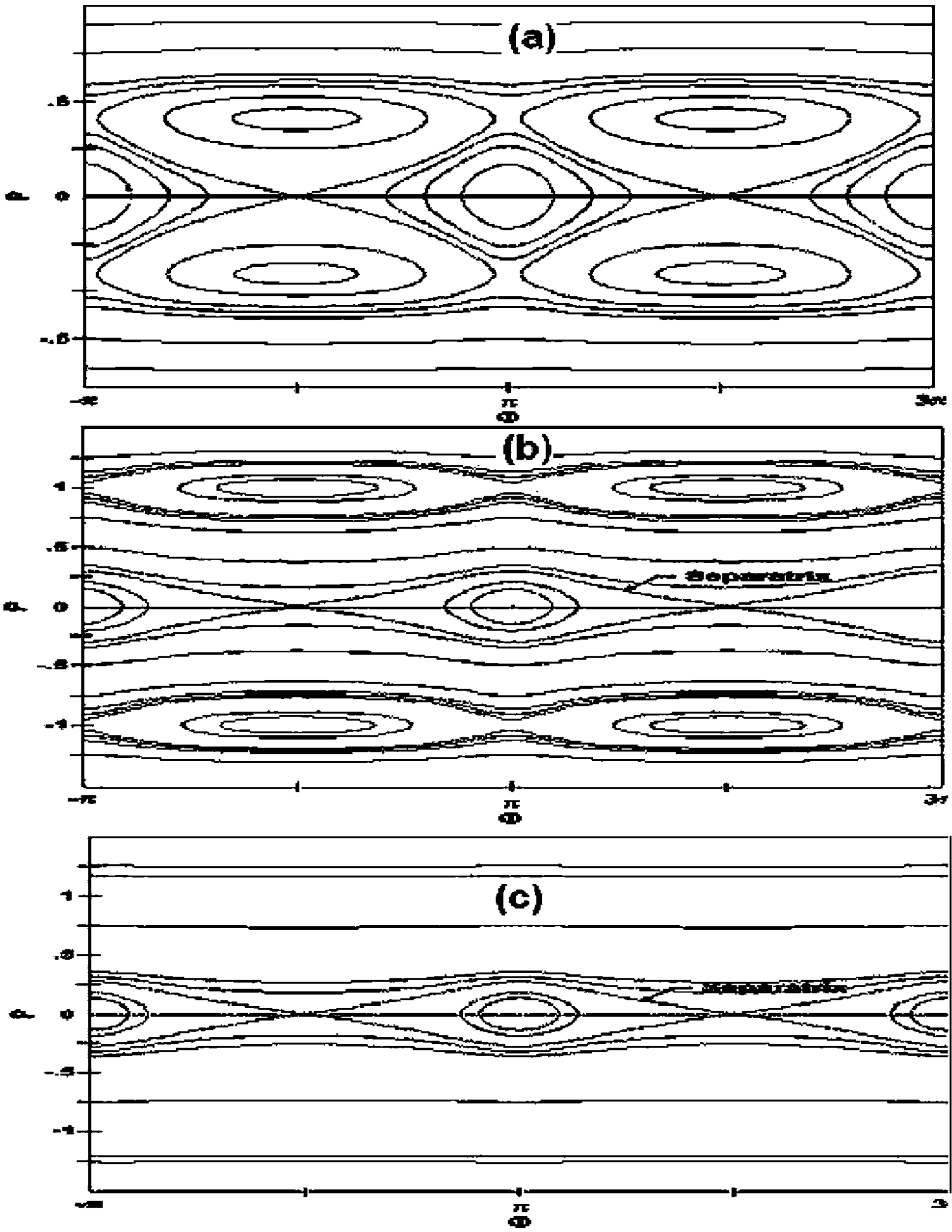

FIG. 3. Phase plane plots of the system, $p=d\phi/ds$ as a function of ϕ, described by the autonomous equation (2.10) with the deformability parameter $r=0.3$, $\nu/C_0=0.0$, and $\lambda=4\times10^{-2}$ and for the following value of the NICC: (a) $C_{nl}/C_0^2=-4/3<C_{nl}^{th}/C_0^2$. Note the absence of the separatrix due to the fact that $C_{nl}<C_{nl}^{th}$. (b) $C_{nl}/C_0^2=-1/3>C_{nl}^{th}/C_0^2$. (**c**) $C_{nl}/C_0^2=4/3>C_{nl}^{th}/C_0^2$.

dispersion while Eq. (2.13) gives the energy at rest of standard RP kink solitons,[4]

$$E_{ks}^{(0)(j)}=8AC_0\omega_0G^{(j)}, \tag{2.14}$$

with

$$G^{(1)}=\frac{1}{(1-\alpha^2)^{1/2}}\tan^{-1}\frac{(1-\alpha^2)^{1/2}}{\alpha}, \tag{2.15}$$

$$G^{(2)}=\frac{\alpha}{(1-\alpha^2)^{1/2}}\tanh^{-1}(1-\alpha^2)^{1/2},$$

and with the pseudowidth

$$d_{ks}^{(1)}=d_0\alpha \quad \text{and } d_{ks}^{(2)}=d_0/\alpha. \tag{2.16}$$

The superscripts (1) and (2) stand for $-1<r\leq 0$ and $0\leq r<1$, respectively.

When the nonlinear coupling term, which corresponds to nonlinear dispersion in Eq. (2.8), is preponderant or when the linear coupling is zero, the kink soliton derived above may become almost compact since they decay in space according to a super-exponential (or double exponential) law as do breather solutions as well (see, e.g., Ref. 21). The characteristic parameters of these kinks usually called kink compactons can be obtained by setting $\nu=C_0=0$ in Eq. (2.8). These kink compactons are not in the scope of this paper. In the next section, the above kink soliton parameters should be of particular importance when determining the different contribution of low-lying excitations including the nonlinear

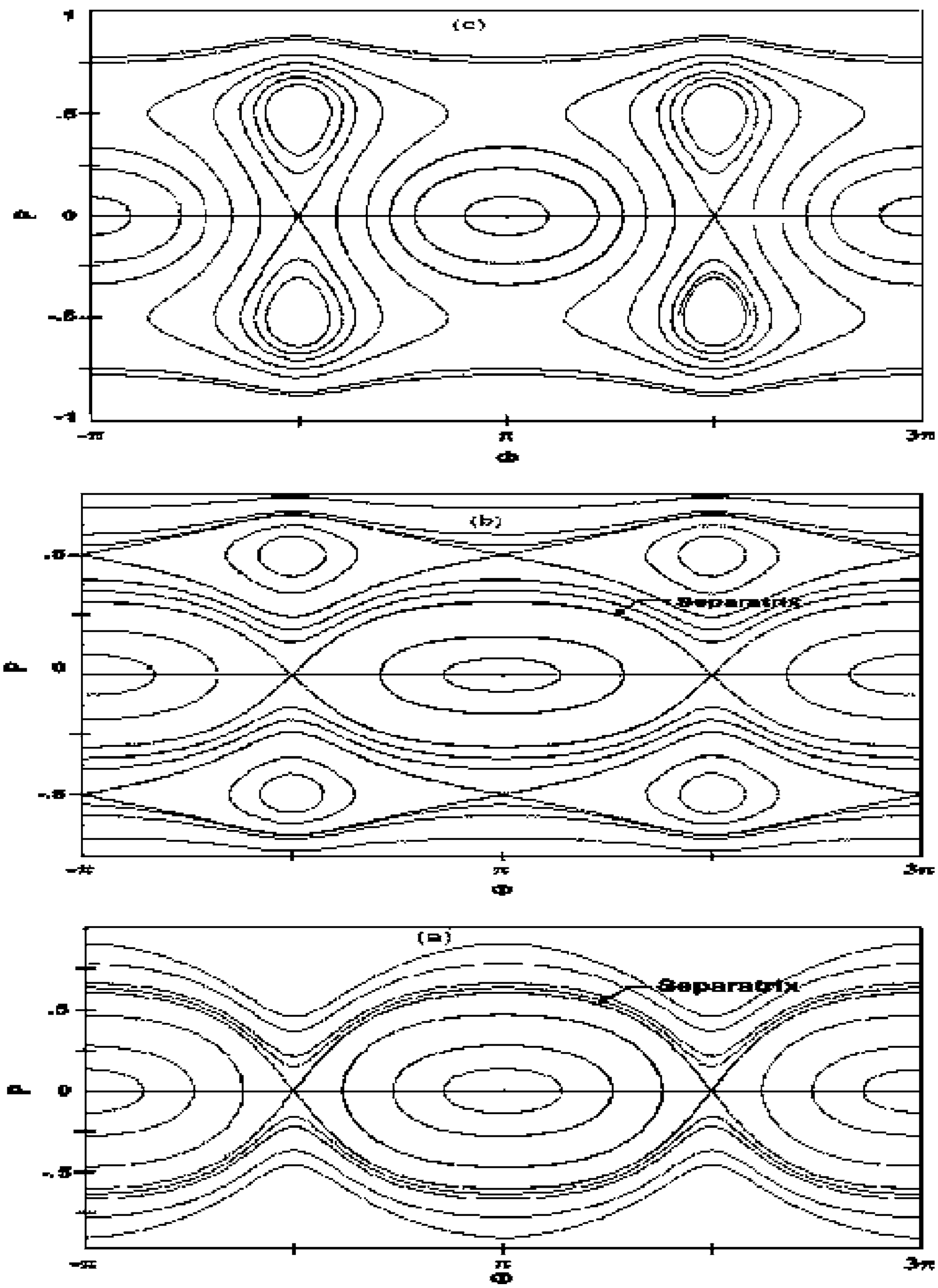

FIG. 4. The same as Fig. 3, but with $r=-0.3$. The phase plane plot remains qualitatively unchanged for changes of the value of the shape parameter r.

solitary waves to the thermodynamic properties of the system.

III. LOW-TEMPERATURE STATISTICAL MECHANICS

In this section, we investigate analytically the low-temperature thermodynamic properties of the model. For this purpose, we use the transfer integral operator (TIO) method to evaluate the classical partition function of the system. The use of the TIO method has the advantage that it gives the exact results without the explicit knowledge of the kink waveform, its internal oscillation and the interactions with other low-lying excitations.

A. Formulation of the TIO method

The thermodynamic quantities of the model are derived from the classical partition function for the discrete system governed by the Hamiltonian (2.1). This partition function can be written in the factored form $Z=Z_{\dot{\phi}}Z_{\phi}$ with $Z_{\dot{\phi}}$ the kinetic contribution given by

$$Z_{\dot{\phi}} = (2\pi A a/\beta h^2)^{N/2}, \tag{3.1a}$$

and Z_{ϕ} the configurational part whose expression is

$$Z_{\phi} = \sum_{n} \exp(-\beta A L \omega_0^2 \varepsilon_n), \tag{3.1b}$$

and where $\beta=1/k_BT$, h is the Planck's constant and $L=Na$ is the total length of the system of N particles with assumed

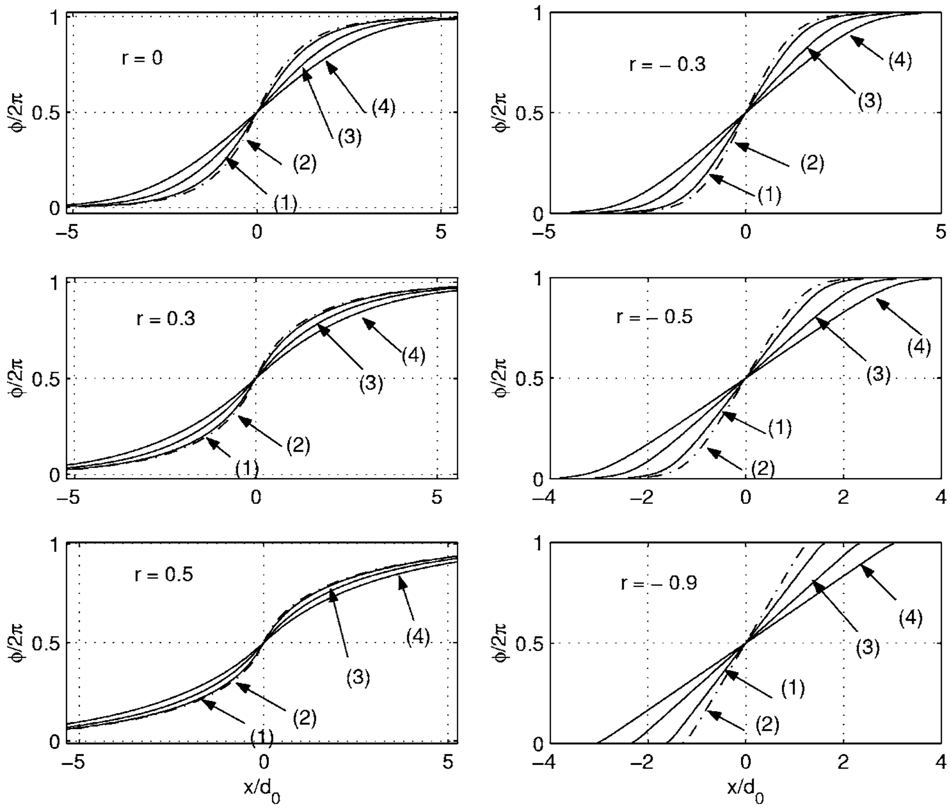

FIG. 5. Kink soliton profiles, obtained from the numerical integration of Eq. (2.12), for different values of the reduced NICC ζ and for few values of the deformability parameter r. The curves in each subplot correspond to the following value of the reduced NICC: (1) $\zeta=0$; (2) $\zeta=-1$; (3) $\zeta=10$, and (3) $\zeta=40$.

periodic boundary condition, $\phi_{N+1}=\phi_1$. The quantities ε_n are the eigenvalues of the TIO defined by

$$\int_{-\infty}^{+\infty} d\phi_i \exp[-\beta A a \omega_0^2 f(\phi_{i+1},\phi_i)]\Psi_n(\phi_i) = \exp(-\beta A a \omega_0^2 \varepsilon_n)\Psi_n(\phi_{i+1}), \quad (3.2a)$$

where

$$f(\phi_{i+1},\phi_i) = \frac{1}{2}\frac{C_0^2}{a^2\omega_0^2}(\phi_{i+1}-\phi_i)^2 + \frac{1}{4}\frac{C_{nl}}{a^4\omega_0^2}(\phi_{i+1}-\phi_i)^4 + \frac{1}{2}[V_{\mathrm{RP}}(\phi_{i+1}) + V_{\mathrm{RP}}(\phi_i)]. \quad (3.2b)$$

This TIO can be approximated, for each specific case, to an equivalent Schrödinger-type equation with eigenfunction $\Psi_n(\phi)$ and eigenvalue ε_n.

B. Continuum limit

In the continuous limit of slowly varying fields, that is $d_0 \gg a$, the transfer integral equation (3.2a) and (3.2b) can be reduced, through a set of transformations and neglecting higher power in (a/d_0), to the following Schrödinger-type equation:

$$-\frac{1}{2m^*}\frac{d^2\Psi_n(\phi)}{d\phi^2} + V_{\mathrm{RP}}(\phi)\Psi_n(\phi) = \tilde{\varepsilon}_n\Psi_n(\phi), \quad (3.3)$$

where $\tilde{\varepsilon}_n=\varepsilon_n-V_0$, with

$$V_0 = -\frac{1}{2\rho}\ln\left(\frac{2\pi a^2}{\rho d_0^2}g_1(y)^2\right), \quad m^* = [\beta A C_0 \omega_0 g_2(y)]^2, \quad (3.4)$$

$$\rho = \beta A a \omega_0^2.$$

For positive values of the NICC C_{nl}, the renormalization factors $g_1(y)$ and $g_2(y)$ are given by

$$g_1(y) = \left(\frac{2y}{\pi}\right)^{1/2} e^y K_{1/4}(y) \quad (3.5)$$

and

$$g_2(y) = \left(\frac{K_{1/4}(y)}{4y[K_{3/4}(y)-K_{1/4}(y)]}\right)^{1/2}. \quad (3.6)$$

Here, $K_\ell(y)$ is the modified Bessel function and the parameter y is related to the NICC C_{nl} through the following relation: $y=\beta A a C_0^4/8C_{nl}$. This parameter may be viewed as the ratio between the IPP energy of the system, $E_0=AaU_0=2AaC_0^4/C_{nl}$, and the Boltzmann energy k_BT, where E_0 is the IPP energy corresponding to a relative displacement $\phi_{i+1}-\phi_i$ for which the contributions of harmonic and anharmonic terms in the IPP are equal. One can then distinguish two different regimes according to whether the Boltzmann energy is less than the characteristic energy E_0 or large compared to E_0. The first results when $y>1/16$, in this case the IPP is dominated by the harmonic term. In the opposite limit ($y<1/16$), the IPP is dominated by the anharmonic term. This means that the renormalization factors $g_1(y)$ and $g_2(y)$ contain all the information concerning the contribution of the

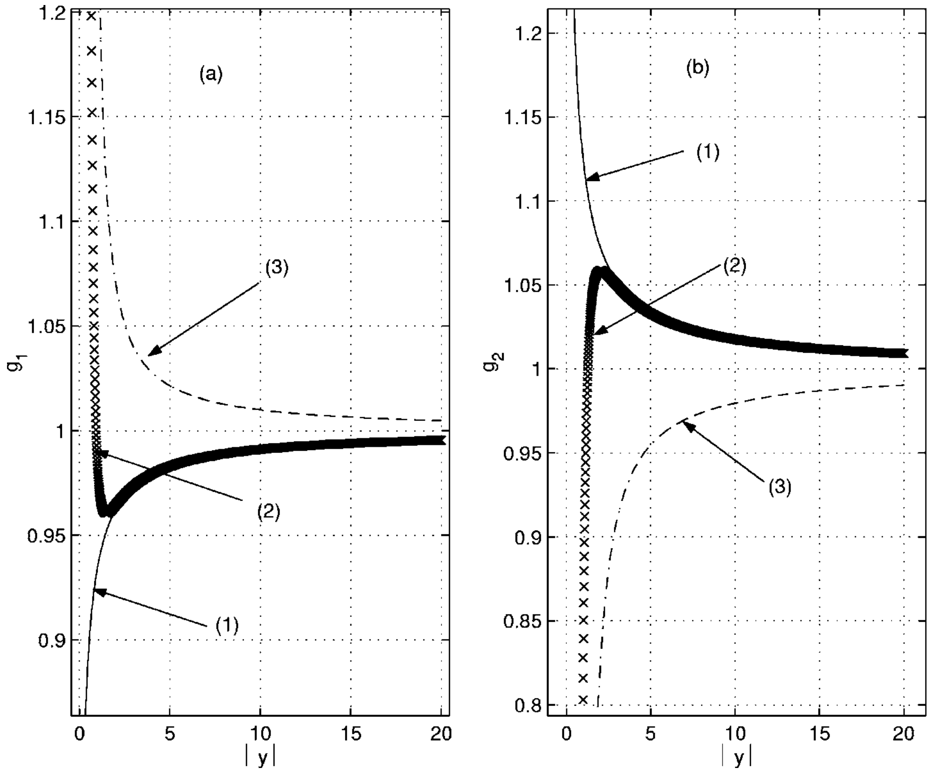

FIG. 6. Renormalization factors (a) $g_1(y)$ and (b) $g_2(y)$ as a function of $|y|$. Curves (1) correspond to the exact result of $g_1(y)$ and $g_2(y)$ while curves (2) stand for the series expansion of $g_1(y)$ given by Eq. (3.28) and $g_2(y)$ given by Eq. (3.29), for positive values of the NICC. It appears that these series expansion reproduce the corresponding exact results if $|y|>2$. Finally, curves (3) stands for negative values of the NICC C_{nl}, $g_1(y)$ and $g_2(y)$ are also approximated by Eq. (3.28) and by Eq. (3.29), respectively.

nonlinear term of the IPP. Figure 6 shows the variation of these factors as a function of the parameter y. It follows that at low temperature, they are close to 1, while for temperature such that $y<1/16$ they become very large evidencing the fact that the system is very sensitive to the anharmonicity of the IPP.

Equation (3.3) is the Schrödinger-type equation for a single particle, where the temperature dependent parameter m^* plays the role of an effective mass, moving in the nonlinear potential $V_{\rm RP}(\phi)$ defined by Eq. (2.3). This equation is identical to the Schrödinger equation obtained for the standard RP model, except the fact that, here, the quantities V_0 and m^* depend on NICC C_{nl} through the renormalization factors. Note that in the limit $C_{nl}\to 0$, that is $y\to +\infty$, $g_1(y)=1$ and $g_2(y)=1$, one recovers the basic results[2,6]

$$V_0 = -\frac{1}{2\rho}\ln\left(\frac{2\pi a^2}{\rho d_0^2}\right) \quad \text{and } m^* = (\beta A C_0 \omega_0)^2. \qquad (3.7)$$

Thus, the Schrödinger equation (3.3) can be solved using the technique usually invoked to solve the Schrödinger type equation obtained for the basic NKG system.

Indeed, in the thermodynamic limit ($L\to\infty$, $N\to\infty$, and $L/N\to$constant), Z_ϕ is dominated by the lowest eigenvalue $\tilde{\varepsilon}_0$. To evaluate $\tilde{\varepsilon}_0$, we use the procedure developed by Croitoru *et al.*[22] and Grecu and Visinescu[23] based on the assumption depending on the large parameter which has the advantage of making a clear distinction between different contributions of low-lying excitations to the thermodynamic properties: phonons, kink, kink-kink interactions, …, etc. Following this procedure, the calculation of the ground state $\tilde{\varepsilon}_0$ is similar to that performed in the case of the standard RP model.[6] Then

$$\tilde{\varepsilon}_0^{(j)} = \tilde{\varepsilon}_{00}^{(j)}(1-4\vartheta^{(j)}), \qquad (3.8)$$

where $\tilde{\varepsilon}_{00}^{(j)}$ is the first term in the asymptotic expansion of the lowest eigenvalue of the isolated potential well given by

$$\tilde{\varepsilon}_{00}^{(1)} = 1/(2\alpha\sqrt{m^*}), \quad \tilde{\varepsilon}_{00}^{(2)} = \alpha/(2\sqrt{m^*}). \qquad (3.9)$$

The quantities $\vartheta^{(j)}$ are the small parameters related to the small shift from the eigenvalue of an isolated well due to the presence of other degenerate minima of the RP potential. The presence of these degenerate minima leads to the tunnel splitting of the lowest level $\tilde{\varepsilon}_{00}^{(j)}$ of the isolated well. The lower extremity can be found from the boundary conditions for the wave function of Eq. (3.3) and its derivatives. The result which takes into account various kink soliton contributions is

$$\vartheta^{(j)} \approx \vartheta_k^{(j)} + \vartheta_{kk}^{(j)}, \qquad (3.10)$$

where $\vartheta_k^{(j)}$ is the single kink soliton contribution given by

$$\vartheta_k^{(j)} = (16\sqrt{m^*}\tilde{C}^{(j)}/\pi)^{1/2}e^{-\varpi^{(j)}}, \qquad (3.11)$$

since, as we shall see below, it is proportional to the single kink soliton energy, and $\vartheta_{kk}^{(j)}$ the kink-kink contribution given by

$$\vartheta_{kk}^{(j)} = -2\vartheta_k^{(j)2}\ln(4\Gamma\varpi^{(j)}\tilde{C}^{(j)}/G^{(j)}), \qquad (3.12)$$

where $\Gamma=1.781\,072\ldots$ is the Euler constant. The quantities $\varpi^{(j)}$ and $\tilde{C}^{(j)}$ are given by

$$\varpi^{(j)} = 8\sqrt{m^*}G^{(j)} = \beta E_{ks}^{(0)(j)}g_2(y) \qquad (3.13)$$

and

$$\tilde{C}^{(1)} = \alpha \exp[2(\sqrt{1-\alpha^2}/\alpha)\tan^{-1}(\sqrt{1-\alpha^2}/\alpha)], \tag{3.14a}$$

$$\tilde{C}^{(2)} = (1/\alpha)\exp(-2\sqrt{1-\alpha^2}\tan^{-1}\sqrt{1-\alpha^2}). \tag{3.14b}$$

From Eqs. (3.8)–(3.11), the lowest eigenvalues $\tilde{\varepsilon}_0$ of the Schrödinger eigenvalue equation is easily obtained,

$$\tilde{\varepsilon}_0^{(j)} = \tilde{\varepsilon}_{00}^{(j)} - 4(16\sqrt{m^*}\tilde{C}^{(j)}/\pi)^{1/2/}\tilde{\varepsilon}_{00}^{(j)} e^{-\varpi^{(j)}} \times[1 - 2(16\sqrt{m^*}\tilde{C}^{(j)}/\pi)^{/1/2}e^{-\varpi^{(j)}}\ln(4\Gamma\varpi^{(j)}\tilde{C}^{(j)}/G^{(j)})]. \tag{3.15}$$

With the knowledge of the eigenvalue $\tilde{\varepsilon}_0$, the classical partition function Z is completely determined and consequently, the thermodynamic quantities can also be evaluated.

Let us begin by calculating the free energy per unit length of the system defined by $f_l=-(1/\beta L)\ln Z$. On the basis of the previous calculation of the thermodynamic properties for the basic NKG, we can separate the free energy into two parts,

$$f_l^{(j)} = f_{ph}^{(j)} + f_{tun}^{(j)}. \tag{3.16}$$

The first part is given by

$$f_{ph}^{(j)} = \frac{1}{\beta a}\ln\left(\frac{\beta\hbar C_0}{a g_1(y)}\right) + \frac{1}{2\beta d_{ks}^{(j)} g_2(y)}, \tag{3.17}$$

and the second part by

$$f_{tun}^{(j)} = -k_B T n_{ks}^{(j)}(1 - B_{ks}^{(j)} n_{ks}^{(j)}), \tag{3.18}$$

with

$$n_{ks}^{(j)} = \frac{2}{d_{ks}^{(j)} g_2(y)}\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{\tilde{C}^{(j)}}{G^{(j)}}\right)^{1/2}\varpi^{(j)1/2}e^{-\varpi^{(j)}} \tag{3.19}$$

and

$$B_{ks}^{(j)} = d_{ks}^{(j)} g_2(y)\ln[4\Gamma\varpi^{(j)}(\tilde{C}^{(j)}/G^{(j)})]. \tag{3.20}$$

When $r=0$(sG), the results (3.16)–(3.20) reduce to those obtained for the sG model.[18] In addition, when the NICC C_{nl} is weak, the first part of the free-energy $f_{ph}^{(j)}$ given by (3.17) can be developed as

$$f_{ph}^{(j)} = \frac{1}{\beta a}\ln(\beta\hbar C_0/a) + \frac{1}{2\beta d_{ks}^{(j)}} + \frac{3}{4}\frac{C_{nl}}{\beta^2 A a^2 C_0^4}\left(1 - \frac{a}{d_{ks}^{(j)}}\right), \tag{3.21}$$

which is in fact the lowest-order terms in series expansion in powers of C_{nl}. The first two terms are the phonon contribution to the free energy of the standard RP model,[6] that is, for $C_{nl}=0$, while the last term is the correction due to the anharmonicity of the IPP. Therefore, Eq. (3.17) can be interpreted as the phonon contributions to the free energy of the system.

Similarly, in the limit $C_{nl}=0$, $g_2(y)=1$, and $\varpi^{(j)}=\beta E_{ks}^{(0)(j)}$, and consequently Eq. (3.19) reduces to the soliton density of the standard RP model within the ideal gas approximation while Eq. (3.20) gives the second virial coefficient.[6,7] This limiting case suggests that one can interpret the expression (3.18) as the contribution of kink soliton in the free energy where $n_{ks}^{(j)}$, given by Eq. (3.19), designates the density. This density can be rewritten in suggestive form as

$$n_{ks}^{(j)} = \frac{2}{d_{\rm eff}^{(j)}}\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{\tilde{C}^{(j)}}{G^{(j)}}\right)^{1/2}(\beta E_{\rm eff}^{(j)})^{1/2}e^{-\beta E_{\rm eff}^{(j)}}, \tag{3.22}$$

where $E_{\rm eff}^{(j)}$ and $d_{\rm eff}^{(j)}$ are the effective kink energy and width given by

$$E_{\rm eff}^{(j)} = E_{ks}^{(0)(j)} g_2(y), \quad d_{\rm eff}^{(j)} = d_{ks}^{(j)} g_2(y). \tag{3.23}$$

Equation (3.23) shows that at finite temperatures, the energy at rest of the kink soliton depends on the temperature and increases with temperature since $g_2(y)$ is an increasing function of the temperature. In addition, $E_{ks}^{0(j)}$ can be viewed as the kink soliton energy at the zero absolute temperature. Note that a similar temperature dependence of the kink soliton energy has been obtained by many authors when studying the quantum statistical mechanics of the basic NKG systems.[24] The dependence on the temperature of the soliton energy has been attributed to the anharmonic interactions between small oscillations since it is induced by the parameter that measures the level of anharmonicity in the system and consequently the strength of interactions. In our case, following these studies, the temperature dependence of the soliton energy is interpreted in the same way as the effect of interaction between small oscillations or phonons; the strength of these interactions being measured by the NICC C_{nl}. In addition, the quantitative effects of these interactions on the kink-soliton parameters (energy and width) are described by the renormalization factor $g_2(y)$. Therefore the anharmonicity in the IPP enhances the energy of creation of kinks and its width and contribute in lowering the kink soliton density in the system. Following the result of the standard RP model,[6] the total density of kink soliton in the system is given by

$$n_s^{(j)} = n_{ks}^{(j)}(1 - B_{ks}^{(j)})n_{ks}^{(j)}, \tag{3.24}$$

where $B_{ks}^{(j)}$ is the second virial coefficient given by Eq. (3.20). This quantity can be rewritten in the more suggestive form depending on the effective kink-soliton parameters as

$$B_{ks}^{(j)} = d_{\rm eff}^{(j)}\ln[4\Gamma\beta E_{\rm eff}^{(j)}(\tilde{C}^{(j)}/G^{(j)})]. \tag{3.25}$$

Following this expression, it appears that, the anharmonicity in the IPP enhances the interactions between kink in the system since the second virial coefficient is an increasing function of C_{nl}.

We now consider another thermodynamic quantity, the specific heat per unit length defined as $c=-T\partial^2 f_1/\partial T^2$. As the free energy, it can be separated into two parts, $c^{(j)}=c_{ph}^{(j)}+c_{tun}^{(j)}$. From Eqs. (3.16)–(3.25), we obtain

$$a c_{ph}^{(j)}/k_B = 1 + \frac{2}{y}\left(\frac{g_1'}{g_1} + \frac{a}{2d_{\rm eff}^{(j)}}\frac{g_2'}{g_2}\right) + \frac{1}{y^2}\left\{\frac{g_1''}{g_1} - \left(\frac{g_1'}{g_1}\right)^2 + \frac{a}{2d_{\rm eff}^{(j)}}\left[\frac{g_2''}{g_2} - 2\left(\frac{g_2'}{g_2}\right)^2\right]\right\} \tag{3.26a}$$

and

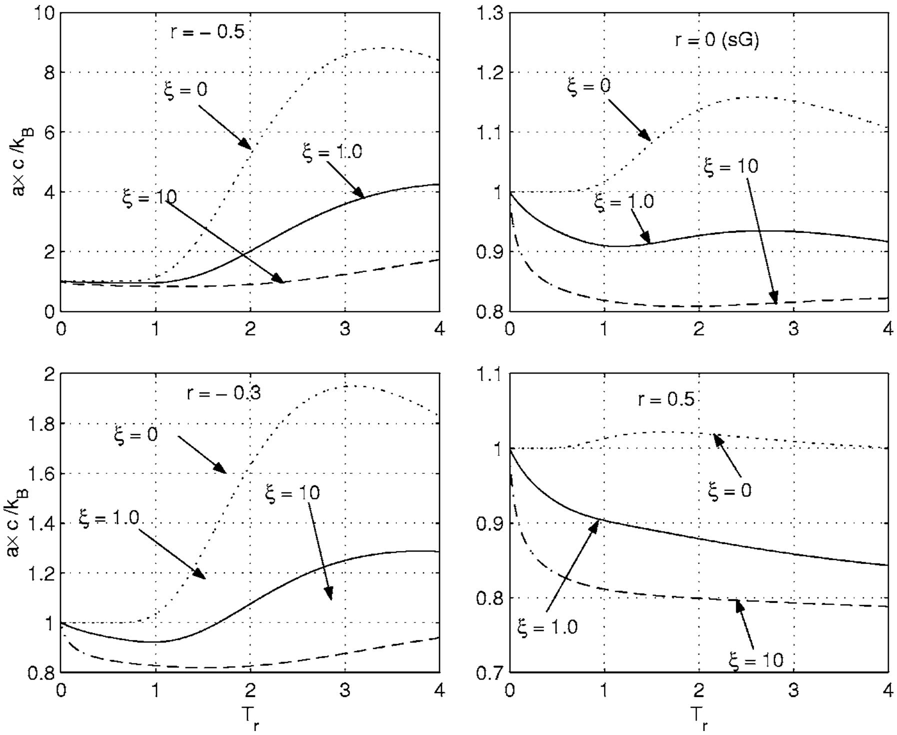

FIG. 7. Specific heat of kink-soliton system as a function of the reduced temperature $T_r = k_B T / A C_0 \omega_0$, for few values of the reduced NICC ζ and for four values of the deformability parameter r.

$$c_{tun}^{(j)}/k_B = n_{ks}^{(j)} \left\{ \left[\left(\beta E_{\text{eff}}^{(j)} - \frac{1}{2} \right) - \frac{1}{y} \frac{g_2'}{g_2} \left(\beta E_{\text{eff}}^{(j)} + \frac{1}{2} \right) \right]^2 - 1 + \frac{1}{2} \left(1 - \frac{1}{y} \frac{g_2'}{g_2} \right) - \frac{1}{y^2} \frac{g_2'}{g_2} \left(\beta E_{\text{eff}}^{(j)} + \frac{1}{2} \right) \right\}, \tag{3.26b}$$

where the prime designates the derivation with respect to $1/y$. In the limit of weak nonlinear coupling C_{nl}, the lowest-order terms in the series expansion in powers of C_{nl} is given by

$$ac^{(j)}/k_B = 1 - \frac{3}{16y} \left(1 - \frac{a}{d_{ks}^{(j)}} \right) + n_{ks}^{(0)(j)} \left[\left(\beta E_{ks}^{(0)(j)} - \frac{1}{2} \right)^2 - \frac{1}{2} \right] - \frac{3}{16y} n_{ks}^{(0)(j)} a \left(\beta E_{ks}^{(0)(j)} + \frac{1}{2} \right) \left[\left(\beta E_{ks}^{(0)(j)} - \frac{1}{2} \right)^2 - \frac{1}{2} \right], \tag{3.27a}$$

where $n_{ks}^{(0)(j)}$ is the kink soliton density of the standard RP model given by

$$n_{ks}^{(0)(j)} = \frac{2}{d_{ks}^{(j)}} \left(\frac{2}{\pi} \right)^{1/2} \left(\frac{\tilde{C}^{(j)}}{G^{(j)}} \right)^{1/2} (\beta E_{ks}^{(0)(j)})^{1/2} e^{-\beta E_{ks}^{(0)(j)}}. \tag{3.27b}$$

When $r=0$, Eqs. (3.27a) and (3.27b) reduce to the results previously obtained for the sG model.[18] The deformability of the system enters in these expressions through the kink soliton parameters; the energy at rest and the width.

The first three terms in the brackets of Eq. (3.26a) and (3.26b) are the contributions, to the specific heat, from the phonon part of the free energy. The first term which is independent of temperature, $1/a$, describes the Dulong-Petit law while the other terms are induced by the anharmonicity of the IPP. The last four terms in the second brackets are the contribution from the second part of the free energy, f_{tun}, in the limit of ideal gas of solitons. Figure 7 shows the influence of anharmonicity of the IPP in the variation of the specific heat as a function of the temperature, in general, the anharmonicity contributes in lowering the specific heat of the system whatever the deformability parameter r. This effect is less important if $y > 2$ and becomes more important for the values of y close or less than $1/16$. This result is understandable since, as pointed out above, for $y > 1/16$, the IPP remains dominated by the harmonic term while for $y < 1/16$ the anharmonic term predominates. Since y depends on the temperature and the NICC C_{nl}, this influence is controlled by the magnitude of the temperature of the system; it is negligible for very low temperature and become more important when the temperature increases and reaches the critical value, depending on the nonlinear coupling coefficient $C_{nl}, T_{cr} = 2AaC_0^4/k_B C_{nl}$. On the other hand, this influence of anharmonicity on the thermodynamic properties and kink soliton parameters is not sensitive to the deformability of the system since there is no coupling between the shape parameter r and the NICC C_{nl}.

We now turn our attention to the case where the NICC has negative values ($C_{nl} < 0$). In this case, the TIO (3.2a) and (3.2b) diverges if $C_{nl} \to -\infty$. However, for weak values of C_{nl}, it is possible to replace it by the Schrödinger equation (3.3) using the cumulant expansion, where V_0, $\tilde{\varepsilon}_n$, and ρ are also given by Eq. (3.4). However the renormalization parameters, $g_2(y)$ and $g_1(y)$, are now given by the series expansion in powers of $1/y$,

$$g_1(y) = 1 - \frac{3}{2^5 y} + \frac{105}{2^{11}y^2} - \frac{3465}{2^{16}y^3} + \frac{675\,675}{2^{23}y^4} + \cdots \tag{3.28}$$

and

$$g_2(y) = 1 + \frac{3}{2^4 y} - \frac{69}{2^9 y^2} + \frac{1647}{2^{13}y^3} - \frac{223\,245}{2^{19}y^4} + \cdots, \tag{3.29}$$

where the parameter y still remains defined by $y=\beta A a C_0^4/8C_{nl}$ as in the preceding paragraph. In order to verify the exactness of expressions (3.28) and (3.29), we have verified successfully that the series expansion of $g_1(y)$ and $g_2(y)$, given by (3.5) and (3.6), respectively, are identical to the series expansion (3.28) and (3.29). Figure 6 confirms this result since the series expansion (3.28) and (3.29) for $C_{nl}>0$ are very close, for $y>2$, to the exact analytical expressions of $g_1(y)$ and $g_2(y)$. This means that the analytical results of the free energy and specific heat derived in the preceding paragraph for $C_{nl}>0$ are also valid for the case $C_{nl}<0$ but with the renormalization factors given by Eqs. (3.28) and (3.29). In addition, the physical signification of y must be revised. Indeed, y is proportional to the ratio between the IPP barrier, $E_1=AaC_0^4/4|C_{nl}|=E_0/8$, and the Boltzmann energy. As in the case of $C_{nl}>0$, we can also distinguish two different situations; according to whether the Boltzmann energy is less than the IPP barrier E_1 or large compared to E_1. When $|y|>1/2$, the barrier height, E_1, is higher than the Boltzmann energy and the particles are confined in the bottom of the potential while for $|y|<1/2$ this barrier height is less than the Boltzmann energy and particles can reach the top of the barrier and escape.

The effective kink parameters, the energy and width, are also given by Eq. (3.25) but the renormalization parameter $g_2(y)$, given by Eq. (3.30), is now a decreasing function of $|C_{nl}|$ and the temperature. Thus, the anharmonicity in the IPP contributes in lowering the energy of creation of kink in the system and then increases the number of thermally activated kink solitons whose expression is given by Eq. (3.23). As in the case of positive C_{nl}, the influence of the anharmonicity is dictated by the magnitude of the temperature. It is negligible for low temperatures and more important for temperatures greater than the critical value $T_{\rm cr}=-AaC_0^4/4k_B C_{nl}$. This influence is not also sensitive to the deformability of the system.

C. Lattice corrections to the free energy of the system

We now consider the lattice corrections to the thermodynamic properties of the model. As pointed out by Trullinger and Sasaki,[25] it is possible, through a set of transformations and neglecting higher powers in $(a/d_0)^2$, that the transfer integral equation (3.2a) and (3.2b) with the first lattice correction included can be approximated by a Schrödinger-type equation. Following this procedure, we obtain the following Schrödinger equation for the TIO (3.2a) and (3.2b):

$$-\frac{1}{2m^*}\frac{d^2\Psi_n(\phi)}{d\phi^2} + V_{\rm eff}(\phi)\Psi_n(\phi) = \tilde{\varepsilon}_n\Psi_n(\phi) \tag{3.30}$$

for a single particle of mass m^* given by Eq. (3.4), moving in the nonlinear effective potential

$$V_{\rm eff}(\phi) = V_{\rm RP}(\phi) - \frac{a^2}{24 d_0^2 g_2(y)^2}\frac{d^2V_{\rm RP}(\phi)}{d\phi^2}, \tag{3.31}$$

where $g_2(y)$ is the renormalization factor defined by Eq. (3.6) for $c_{nl}>0$ and by the series expansion (3.29) for $C_{nl}<0$. The eigenvalues $\tilde{\varepsilon}_n$ of this Schrödinger equation is related to the eigenvalues ε_n of the TIO (3.2a) and (3.2b) through the relation $\tilde{\varepsilon}_n=\varepsilon_n-V_0$, where V_0 is given by Eq. (3.4) and where $g_1(y)$ is given by Eq. (3.5) for $C_{nl}>0$ and by the series expansion (3.28) for $C_{nl}<0$.

As one can easily see, the Schrödinger equation (3.30) is identical to that obtained at order (a/d_0), that is in the continuum limit, except for the fact that the potential $V_{\rm RP}(\phi)$ is replaced here by the effective potential (3.31) depending both on the substrate potential $V_{\rm RP}(\phi)$ and on the scaling parameter $g_2(y)$. Therefore, we can use the procedure of the preceding paragraph to solve $\tilde{\varepsilon}_0$. Following this procedure, the ground state $\tilde{\varepsilon}_0$ is given by

$$\tilde{\varepsilon}_0^{(j)} = \tilde{\varepsilon}_{00}^{(j)}(1-4\vartheta^{(j)})(1-\Lambda^{(j)}), \tag{3.32}$$

where $\tilde{\varepsilon}_{00}^{(j)}$ is the first term in the asymptotic expansion of the lowest eigenvalue of the isolated potential well given by Eq. (3.9) and

$$\Lambda^{(j)} = (1/24)(a^2/d_{\rm eff}^{(j)2}). \tag{3.33}$$

The expression of the small parameters $\vartheta^{(j)}$ which takes into account kink and kink-kink contributions is

$$\vartheta^{(j)} \approx \vartheta_k^{(j)} + \vartheta_{kk}^{(j)}, \tag{3.34}$$

where $\vartheta_k^{(j)}$ is the single kink solition contribution given by

$$\vartheta_k^{(j)} = (16\sqrt{m^*}\tilde{C}^{(j)}/\pi)^{1/2}(1-\Lambda^{(j)}/3)e^{-\varpi^{(j)}}, \tag{3.35}$$

and $\vartheta_{kk}^{(j)}$ the kink-kink contribution given by

$$\vartheta_{kk}^{(j)} = -2\vartheta_k^{(j)2}[\ln(4\Gamma\varpi^{(j)}\tilde{C}^{(j)}/G^{(j)}) - (2/3)\Lambda^{(j)}], \tag{3.36}$$

with Γ the Euler constant, and $\tilde{C}^{(j)}$ given by Eq. (3.14). The quantities $\varpi^{(j)}$ are given as

$$\varpi^{(j)} = \beta E_{\rm eff}^{(j)}(1-\Lambda^{(j)}/3), \tag{3.37}$$

where $E_{\rm eff}^{(j)}$ is the effective kink soliton energy in the continuum limit. From Eqs. (3.32)–(3.37), the lowest eigenvalues $\tilde{\varepsilon}_0$ of the Schrödinger eigenvalue equation can be easily obtained and then the expression of the classical partition can be followed. Thus, the free energy per unit length is given by

$$f_l^{(j)} = f_{ph}^{(j)} + f_{tun}^{(j)}, \tag{3.38}$$

where the phonon contribution is given by

$$f_{ph}^{(j)} = \frac{1}{\beta a}\ln(\beta\hbar C_0/a) + \frac{1}{2\beta d_{\text{eff}}^{(j)}}\left(1 - \frac{a^2}{24 d_{\text{eff}}^{(j)2}}\right), \quad (3.39)$$

and the kink soliton contribution,

$$f_{tun}^{(j)} = -k_B T n_{c\_ks}^{(j)}(1 - B_{c\_ks}^{(j)} n_{c\_ks}^{(j)}). \quad (3.40)$$

The quantity $n_{c\_ks}^{(j)}$ is the lattice corrected kink soliton density within the ideal gas approximation,

$$n_{c\_ks}^{(j)} = \frac{2}{d_{\text{eff}}^{(j)}}\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{\tilde{C}^{(j)}}{G^{(j)}}\right)^{1/2}\left(1 - \frac{a^2}{72 d_{\text{eff}}^{(j)2}}\right)(\beta E_{c\_\text{eff}}^{(j)})^{1/2} e^{-\beta E_{c\text{-eff}}^{(j)}}, \quad (3.41)$$

with

$$E_{c\_\text{eff}}^{(j)} = E_{\text{eff}}^{(j)}\left(1 - \frac{a^2}{72 d_{\text{eff}}^{(j)2}}\right), \quad (3.42)$$

the corrected kink effective energy due to lattice discreteness, while $B_{c\_ks}^{(j)}$, given by

$$B_{ks}^{(j)} = d_{\text{eff}}^{(j)}\left(1 + \frac{1}{24}\frac{a^2}{d_{\text{eff}}^{(j)2}}\right)\left(\ln[4\Gamma\beta E_{c\_\text{eff}}^{(j)}(\tilde{C}^{(j)}/G^{(j)})] - \frac{1}{36}\frac{a^2}{d_{\text{eff}}^{(j)2}}\right), \quad (3.43)$$

is the lattice corrected second virial coefficient. The corrected effective energy is therefore, as expected, lowered below the continuum zero-order value. The discreteness corrections appearing in Eq. (3.42) for the kink soliton rest energy can be interpreted as a downward renormalization of the kink soliton creation energy in this discrete system. In the limit $(a/d_0)^2 \to 0$, Eqs. (3.39)–(3.43) reduce to those obtained in the continuum limit, namely Eqs. (3.17)–(3.20). In addition, when $r=0$ they reduce to the results previously obtained for the sG model.[19] The above corrected expressions depend not only on the characteristic length of the system d_0, the shape of the substrate potential but also on the anharmonicity of the IPP through the effective kink width $d_{\text{eff}}^{(j)}$ defined by Eq. (3.23). This dependence of the lattice corrections factors to the kink soliton effective width is at the origin of the temperature dependence of the first lattice corrections to the thermodynamic quantities of the system.[19] As mentioned above, the temperature dependence of kink soliton effective parameters, which results from the anharmonicity of the IPP, may be attributed to the anharmonicity of the interactions between linear phonons. Note also that, the analytical expressions (3.39)–(3.43) suggest that, for positive values of the NICC C_{nl}, the first lattice corrections become less and less important when the temperature is increased while for negative values of C_{nl} they are more and more important for increasing temperatures.

IV. CONCLUSION

In this paper, we have investigated the low-temperature statistical mechanics of the nonlinear Klein-Gordon (NKG) model with the Remoissenet-Peyrard substrate potential and anharmonic interparticle pair potential (IPP). We have used the phase plane plot to predict that the system may sustain different features concerning the existence of excitations: For convex IPP obtained for positive nonlinear interparticle coupling coefficient (NICC), the system exhibits the kink and phonons excitations usually observed in the basic NKG system. However, for nonconvex IPP obtained for negative values of the NICC, the anharmonicity of the IPP is at the origin of the appearance of new types of excitations and may be also responsible for the disintegration of kink solitons if the value of the NICC is lower than a particular threshold. It should be mentioned that these results are qualitatively independent of the deformability of the system.

We have calculated also the thermodynamic properties of the system by means of the TIO method associated with the asymptotic methods from the theory of differential equations depending on a large parameter. The free energy and the heat capacity of the system exhibiting kink solitons have been exactly calculated. Due to the anharmonicity of the IPP, the obtained results are renormalized by the factors which depend both on the NICC and on the temperature, but not on the deformability parameter. Furthermore, and contrary to we can naively expect, the soliton effective parameters (energy of creation and width) are also corrected by these temperature dependent renormalization factors. The analysis shows that at very low temperatures, the quantitative effects of the anharmonicity of the IPP to the thermodynamic quantities are very small and can be neglected, and become large for temperatures close to or exceeding some critical values. Thus, due to this coupling between the NICC and the temperature of the system, the quantitative effects of the anharmonicity of the IPP to the thermodynamic quantities and kink to the soliton effective parameters are controlled by temperature. In addition, the analysis of the discreteness factor resulting from the first lattice corrections to the free-energy shows that the magnitude of the discreteness effects is monitored by temperature and the deformability parameter of the system.

The present results allow one to predict three things. (i) The kink soliton parameters (energy and width) of the basic NKG models give the zero-temperature parameters of kink solitons in the corresponding NKG models with anharmonic IPP. In addition, these zero-temperature parameters set the scale of the corresponding parameters in the NKG model with anharmonic IPP. (ii) As far as the statistical mechanics of the NKG model with anharmonic IPP is concerned, parameters of kink solitons of this model are temperature dependent. (iii) The renormalization factors resulting from the first lattice corrections to the thermodynamic properties and to the static kink energy are temperature dependent for the kink soliton bearing systems with anharmonic IPP and are also sensitive to the deformability parameter of the system.

As previously mentioned,[18] although a complete proof of a similar CKBT phenomenology does not exist at present, our results strongly support the idea that their phenomenology is valid at low temperatures. This comes from the phonon part which reproduces exactly, for weak anharmonicity, the specific heat capacity of a phonon lattice gas. We hope that, these exact results for one-dimensional NKG systems with anharmonic interparticle interactions will stimulate further with the goal of making detailed comparisons to test the validity of the phenomenological generalization of the CKBT theory.

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[1] A. C. Scott, *Nonlinear Science: Emergence and Dynamics of coherent structures*, (Oxford University Press, Oxford, 1999).

[2] J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **22**, 477 (1980).

[3] A. M. Dikandé and T. C. Kofané, J. Phys.: Condens. Matter **3**, 5203 (1991); Solid State Commun. **89**, 559 (1994); P. Tchofo Dinda, Phys. Rev. B **46**, 12012 (1992).

[4] M. Remoissenet and M. Peyrard, J. Phys. C **14**, L481 (1981); M. Peyrard and M. Remoissenet, Phys. Rev. B **26**, 2886 (1982).

[5] T. Tsuzuki and K. Sasaki, Prog. Theor. Phys. **94**, 73 (1988).

[6] D. Yemélé and T. C. Kofané, Phys. Rev. B **56**, 3353 (1997).

[7] D. Yemélé and T. C. Kofané, Phys. Rev. B **62**, 5277 (2000).

[8] Y. S. Kivshar, Phys. Rev. E **48**, R43 (1993).

[9] F. Zhang, Phys. Rev. E **54**, 4325 (1996).

[10] F. Motross and H. Büttner, J. Phys. C **16**, 4539 (1983).

[11] P. Rosenau and J. M. Hyman, Phys. Rev. Lett. **70**, 564 (1993).

[12] S. Dusuel, P. Michaux, and M. Remoissenet, Phys. Rev. E **57**, 2320 (1998).

[13] P. Tchofo Dinda and M. Remoissenet, Phys. Rev. E **60**, 6218 (1999).

[14] M. A. Aguero M. J. Paulin, Phys. Rev. E **63**, 046606 (2001).

[15] P. Tchofo Dinda, T. C. Kofané, and M. Remoissenet, Phys. Rev. E **60**, 7525 (1999).

[16] P. Tchofo Dinda, T. C. Kofané, and M. Remoissenet, Phys. Rev. E **60**, 7525 (1999).

[17] A. S. Tchakoutio Nguetcho, J. R. Bogning, D. Yemélé, and T. C. Kofané, Chaos, Solitons Fractals **21**, 165 (2004).

[18] D. Yemélé and T. C. Kofané, J. Phys. A **37**, 8697 (2004).

[19] D. Yemélé and T. C. Kofané, J. Phys.: Condens. Matter **17**, 1747 (2005).

[20] A. Hasan Nayfeh, *Perturbation Methods* (Wiley, New York, 1973).

[21] B. Dey, M. Eleftheriou, S. Flach, and G. P. Tsironis,, Phys. Rev. E **65**, 017601 (2001).

[22] M. Croitoru, D. Grecu, A. Visinescu, and V. Cionga, Rev. Roum. Phys. **22**, 853 (1984).

[23] D. Grecu and A. Visinescu, J. Phys. I **3**, 1541 (1993).

[24] K. Maki and H. Takayama, Phys. Rev. B **20**, 3223 (1979).

[25] S. E. Trullinger and K. Sasaki, Physica D **28**, 181 (1987).