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Temperature dependence of first lattice corrections to the free-energy of kink compacton-bearing systems

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Abstract
The free-energy of discrete nonlinear Klein–Gordon (NKG) systems with anharmonic interparticle interactions is derived by means of the transfer integral operator method, with the first lattice corrections and kink–kink interactions taken into account. Two particular substrate potentials are considered: the $\phi - four$ and the sine-Gordon (sG). We show that, in the general case where the system exhibits the kink soliton like excitations, the correction factors, due to the lattice discreteness, appearing in the free-energy and in the lattice corrected static kink soliton energy, depend on the temperature through a coupling of the interparticle anharmonicity strength to the temperature. Similarly, in the purely anharmonic NKG systems, characterized by the absence of the linear dispersion, where thermodynamic properties are sensitive to kink compactons, we find also that the correction factors are temperature dependent. In both cases, they decrease with increasing temperatures, although the correction factors verify different temperature laws.

1. Introduction

The properties of a wide variety of systems of condensed matter physics can be understood in terms of nonlinear excitations (kinks) which arise as a solution of equations of the nonlinear Klein–Gordon (NKG) type [1]. These systems are divided into two main parts. In one part, continuous systems are treated as fluids and plasmas, and kinks arise as solution of partial differential equations. In the other part, intrinsically discrete systems are considered such as anharmonic atomic lattices, chains of magnetic ions and hydrogen-bonded chains. Here, the dynamics of the system can be modelled by the differential-difference equations or discrete NKG equation which cannot be solved exactly. Except in some particular cases, for example the Toda lattice [2], which is known to be completely integrable, the models proposed are usually treated in the displacive limit where the continuum approximation is valid, assuming a slow variation of the scalar field with space. However, this is not always the case and solitons with a width of a few lattice spacings have been observed [3]. This continuum approximation obtained by ignoring the discrete structure with the lattice soliton yields results that are quantitatively and/or qualitatively inaccurate according to whether the soliton width is of the order of the lattice constant or large compared to the lattice spacing. In the first case, the system is weakly discrete, while in the second case the system is highly discrete.

The influence of lattice discreteness on the properties of nonlinear systems that are governed by these equations of the NKG type has been investigated by several authors [4–12]. These studies have pointed out a large variety of effects ranging from correction of the continuum solutions (weakly discrete system) to completely different phenomena which do not appear in the continuum limit (highly discrete case), namely, the modification of kink velocity and shape, and the pinning of kinks on the lattice.

Similarly, the statistical mechanics of the discrete NKG systems, which is a particularly important problem in condensed matter physics, has also been investigated. In fact, Currie *et al* [13] have developed an ideal-gas phenomenology for continuum NKG systems based on the particle like behaviour of dilute kinks. They found agreement between thermodynamic quantities obtained phenomenologically and calculated by the exact transfer integral operator (TIO) method. Both ideal-gas phenomenology and the TIO method [14, 15] have been extended to include kink–kink interactions [16, 17] and lattice effects [18–21] to the thermodynamic properties of the system.

However, special attention has been paid only to the basic NKG systems, i.e., for models which are equivalent to a linear chain of particles harmonically coupled with the nearest neighbours and subjected to an on-site potential which possesses several degenerate minima. This spatial degeneracy associated with the linear coupling between lattice sites is then at the origin of a kink structure with infinite wings, which causes mutual interactions between adjacent kinks. This is the merit of Rosenau and Hyman [22], who investigated a special type of Korteweg–de Vries equation to discover that solitary waves may become compact in the presence of a nonlinear dispersion. Such solitary waves, which are characterized by a compact support, i.e., the absence of infinite tail, have been called compactons. Since this pioneering work, the existence and the dynamics of compactons in the nonlinear systems have become the subjects of many works [23–31]. For example, Kivshar [23] reported that intrinsic localized modes in purely anharmonic lattices may exhibit compacton like properties. Similarly, Dusuel *et al* [25] demonstrated that the same phenomenology can also appear in NKG systems with anharmonic coupling, and then obtained the experimental evidence of the existence of static kink compactons in a real system made up by identical pendulums connected by anharmonic springs. The study of lattice effects on the motion of this kink compacton [28] has revealed that the effects of lattice discreteness and the presence of a linear coupling between lattices sites are detrimental to a stable ballistic propagation of the compacton because of the particular structure of the small oscillation frequency spectrum of the compacton in which the lower frequency internal modes enter in direct resonance with phonons modes. Recently [32], by means of the TIO method we have derived the thermodynamic properties of this system. We have shown that the presence of kink compactons in the thermodynamic properties of the system is signalled by a term proportional to $\exp[-\chi(\beta E_{\mathrm{kc}}^{(0)})^{3/4}]$, where $E_{\mathrm{kc}}^{(0)}$ is the energy of the static kink compacton and χ, a temperature-independent coefficient, instead of the well-known relation $\exp(-\beta E_s^{(0)})$, where $E_s^{(0)}$ is the energy of the static kink valid for the kink solitons of the basic NKG systems.

Our purpose in this paper is to extend the investigation of [32] on the calculation of the thermodynamic properties of NKG systems supporting kink compactons in order to include the lattice effects. Our results are valid for weakly discrete system, i.e., for the case where the kink width is large compared to the lattice spacing and where the effect of pinning of kinks is so small that the trapping of the kink in the pinning potential well plays a minor role.

The paper is organized as follows. Section 2 deals with the model description. The 1D Hamiltonian of the NKG model with anharmonic coupling is presented and the characteristic parameters, of the kink compacton like excitation solution of the resulting generalized NKG equation, are derived for two particular on-site potentials: the $\phi - four$ and the sine-Gordon (sG) potentials. In addition, the energy of a kink soliton in the limit of weak nonlinear coupling is also calculated. In section 3, we use the TIO method to derive the different contributions of low-lying excitations (phonons, kink and kink–kink) in the expression of the free-energy which takes into account the lattice corrections and from which other thermodynamic quantities can be explicitly derived. We find that the lattice corrections are a function of the temperature. Two distinct cases are considered: at first, the case where the systems exhibit static kink soliton like excitation and next, the case where they rather exhibit static kink compacton, i.e., the case of purely anharmonic systems. Finally, section 4 provides a summary and concluding remarks.

2. Model and kink excitations

We consider a one-dimensional (1D) chain of N particles with mass m, anharmonically coupled to their nearest neighbours, and subjected to a nonlinear on-site potential $V_s(\phi)$. The Hamiltonian of this discrete chain may be written as

$$H = \sum_i Aa \left\{ \frac{1}{2}\left(\frac{\mathrm{d}\phi_i}{\mathrm{d}t}\right)^2 + \frac{C_0^2}{2a^2}(\phi_{i+1}-\phi_i)^2 + \frac{C_{nl}}{4a^4}(\phi_{i+1}-\phi_i)^4 + \omega_0^2 V_s(\phi_i) \right\}, \tag{1}$$

where ϕ_i denotes the dimensionless displacement of the ith particle measured from the ith lattice site. The constants C_0 and ω_0 are the characteristic velocity and frequency, respectively, and the factor $A \approx ma$ sets the energy scale of the system. The positive parameter C_{nl} controls the strength of the nonlinear interparticle coupling. The last term of equation (1) is the substrate potential which has at least two degenerate minima. In this paper, we consider two particular cases: the $\phi - four$ potential $V_s(\phi) = (1/8)(1-\phi^2)^2$, and the sine-Gordon (sG) potential $V_s(\phi) = 1 - \cos(\phi)$. When $C_{nl} = 0$, the Hamiltonian (1) reduces to the well-known NKG system Hamiltonian previously used by Currie, Krumhansl, Bishop, and Trullinger (CKBT) [13].

The characteristic length of this generalized NKG system (1) is given by $d_0 = C_0/\omega_0$. However, in the purely anharmonic case characterized by the absence of the harmonic term ($C_0 = 0$) in equation (1), the new characteristic length of the system becomes

$$d_{\mathrm{kc}} = \pi(6C_{nl}/\eta\omega_0^2)^{1/4}, \tag{2}$$

where $\eta = 1$ for the $\phi - four$ potential and $\eta = 8$ for the sG one. Thus, as we shall see below, d_0 characterizes the kink soliton systems while d_{kc} stands for the characteristic length for the kink compacton systems. In both cases, two different regimes can occur according to whether the characteristic length of the system is of the order of the lattice constant a or large compared to a. The first situation results when the interaction energy between neighbours is small compared to the on-site potential. In this case we are faced with the discrete system. The opposite situation ($d_0 \gg a$ or $d_{\mathrm{kc}} \gg a$) occurs when the linear coupling and nonlinear coupling between sites are strong enough to ensure that the variation of ϕ_i from site to site is quite small and one can use the standard continuum approximation $\phi_i(t) \rightarrow \phi(x,t)$ and expand $\phi_{i\pm1}$

around ϕ_i, with $x = ia$. Under these conditions, the Hamiltonian (1) is transformed to

$$H = A\int \mathrm{d}x \left\{ \frac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2 + \frac{C_0^2}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{C_{nl}}{4}\left(\frac{\partial\phi}{\partial x}\right)^4 + \omega_0^2 V_s(\phi)\right\}. \tag{3}$$

We shall have the occasion to use both forms, (1) and (3), of the Hamiltonian of the system. The discrete form (1) is used in obtaining exact statistical mechanical results via the TIO formalism, whereupon the explicit process of taking the continuum limit follows. The continuum form (3) 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 equation (3):

$$\frac{\partial^2\phi}{\partial t^2} - C_0^2\frac{\partial^2\phi}{\partial x^2} - 3C_{nl}\left(\frac{\partial\phi}{\partial x}\right)^2\frac{\partial^2\phi}{\partial x^2} + \omega_0^2\frac{\mathrm{d}V_s(\phi)}{\mathrm{d}\phi} = 0. \tag{4}$$

In order to find, as usual, travelling waves at velocity v, we use the independent variable $s = x - vt$. Thus, equation (4) is transformed to

$$\left(v^2 - C_0^2\right)\frac{\mathrm{d}^2\phi}{\mathrm{d}s^2} - 3C_{nl}\left(\frac{\mathrm{d}\phi}{\mathrm{d}s}\right)^2\frac{\mathrm{d}^2\phi}{\mathrm{d}s^2} + \omega_0^2\frac{\mathrm{d}V_s(\phi)}{\mathrm{d}\phi} = 0. \tag{5}$$

This equation admits different kinds of excitations [25, 29, 32] among which are the kink excitations. These kinks are the localized structure of permanent profile and verify the boundary conditions $\lim_{x\to\pm\infty}\phi = \pm 1$ and $\lim_{x\to\pm\infty}\mathrm{d}\phi/\mathrm{d}x = 0$ for the $\phi - four$ potential, and $\lim_{x\to\pm\infty}\phi = 0(2\pi)$ and $\lim_{x\to\pm\infty}\mathrm{d}\phi/\mathrm{d}x = 0$ for the sG potential. Within these conditions, the first integral resulting from equation (5) is given by

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}s}\right)^4 + \frac{2}{3}\frac{C_0^2}{C_{nl}\gamma_{\mathrm{L}}^2}\left(\frac{\mathrm{d}\phi}{\mathrm{d}s}\right)^2 - \frac{4}{3}\frac{C_0^2}{C_{nl}d_0^2}V_s(\phi) = 0, \tag{6}$$

where $\gamma_{\mathrm{L}} = (1 - v^2/C_0^2)^{-1/2}$ is the Lorentz factor. Thus, by solving equation (6), it is easy to show that the shape of the kink soliton structure is described by the following implicit integral equation:

$$\int_{\phi(s_0)}^{\phi(s)} \frac{\mathrm{d}\phi}{2\sqrt{V_s(\phi)}}\left(1 + \sqrt{1 + 12\frac{C_{nl}\gamma_{\mathrm{L}}^4}{C_0^2 d_0^2}V_s(\phi)}\right)^{1/2} = \pm\frac{\gamma_{\mathrm{L}}}{d_0}(s - s_0), \tag{7}$$

while its energy is given by

$$E_{\mathrm{ks}} = 2AC_0\omega_0\gamma_{\mathrm{L}}\int_{\phi_{01}}^{\phi_{02}} \mathrm{d}\phi\sqrt{V_s(\phi)}\frac{1 + 4\frac{C_{nl}\gamma_{\mathrm{L}}^2}{C_0^2 d_0^2}V_s(\phi) + \sqrt{1 + 12\frac{C_{nl}\gamma_{\mathrm{L}}^4}{C_0^2 d_0^2}V_s(\phi)}}{\left(1 + \sqrt{1 + 12\frac{C_{nl}\gamma_{\mathrm{L}}^4}{C_0^2 d_0^2}V_s(\phi)}\right)^{3/2}}, \tag{8}$$

where ϕ_{01} and ϕ_{02} are the positions of two adjacent degenerate minima of the substrate potential: $\phi_{01} = -1$ and $\phi_{02} = 1$ for the $\phi - four$ potential, and $\phi_{01} = 0$ and $\phi_{02} = 2\pi$ for the sG potential. $\phi(s_0)$ is the value of the displacement field ϕ at the centre of mass of kink soliton. From symmetry considerations, $\phi(s_0)$ is taken as the position of the potential barrier separating the two adjacent minima: $\phi(s_0) = 0$ for the $\phi - four$ potential and $\phi(s_0) = \pi$ for the sG potential. Figures 1 and 2 show the influence of the anharmonic interparticle term on the kink soliton profile. These shapes have being obtained from the numerical integration of equation (7). It follows that the shape of kink solitons is weakly modified by the presence of the anharmonic interparticle term. When the interparticle anharmonicity strength C_{nl} is weak, the expression of the energy (8) can be easily integrated. To first order in C_{nl}, one obtains:

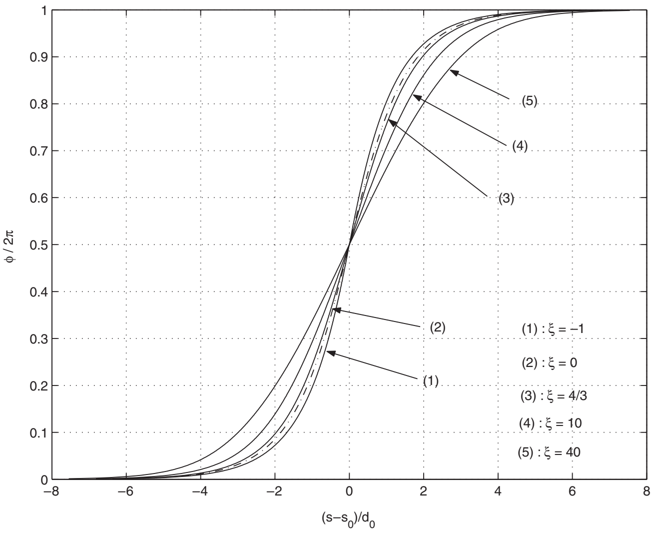

Figure 1. Kink soliton profile, for the $\phi - four$ potential, for a few values of the dimensionless interparticle anharmonicity strength $\xi = C_{nl}/C_0^2$.

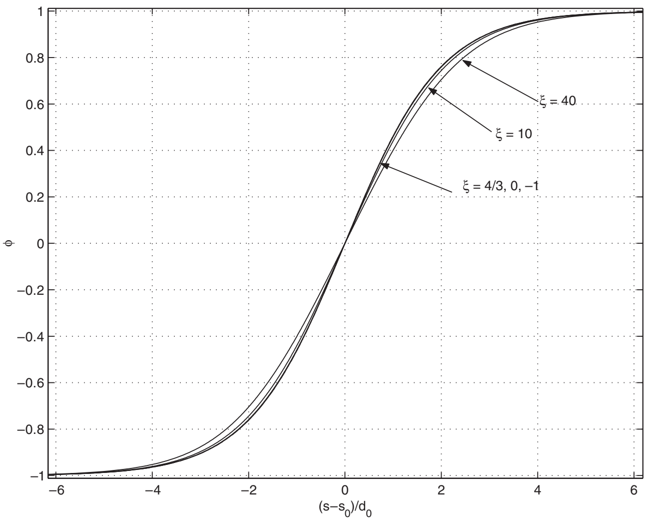

Figure 2. Kink soliton profile, for the sG potential, for a few values of the dimensionless interparticle anharmonicity strength $\xi = C_{nl}/C_0^2$.

- for the $\phi - four$ potential,

$$E_{\mathrm{ks}} = E_s^{(0)}\gamma_{\mathrm{L}}\left[1 + \frac{3}{70}\frac{C_{nl}\gamma_{\mathrm{L}}^2}{C_0^2 d_0^2}\left(4 - 3\gamma_{\mathrm{L}}^2\right)\right], \qquad \text{with } E_s^{(0)} = \tfrac{2}{3}AC_0\omega_0, \tag{9}$$

- for the sG potential,

$$E_{\mathrm{ks}} = E_s^{(0)}\gamma_{\mathrm{L}}\left[1 + \frac{2}{3}\frac{C_{nl}\gamma_{\mathrm{L}}^2}{C_0^2 d_0^2}\left(4 - 3\gamma_{\mathrm{L}}^2\right)\right], \qquad \text{with } E_s^{(0)} = 8AC_0\omega_0, \tag{10}$$

where $E_s^{(0)}$ is the well-known rest energy of the kink soliton in the basic NKG system. It appears from equations (9) and (10) that, in the non-relativistic regime ($\gamma_{\mathrm{L}} = 1$), the correction term induced by the presence of the anharmonic interparticle term increases with the increasing values of C_{nl} and remains very small for weak values of C_{nl}.

As previously mentioned [25], these kink solitons may become compact if, in equation (5), the nonlinear coupling term, which corresponds to the nonlinear dispersion, is preponderant:

the linear coupling term can be zero. In this limit, $v = C_0 = 0$, the kink compacton structure has the following explicit expression [25, 32]:

- for the $\phi - four$ potential,

$$\phi(s) = \sin\left[(s - s_0)\pi/d_{\rm kc}\right], \qquad \text{for } |(s - s_0)| < d_{\rm kc}/2, \tag{11}$$

with $\phi(s) = -1$ for $(s - s_0) < -d_{\rm kc}/2$ and $\phi(s) = +1$ for $(s - s_0) > d_{\rm kc}/2$,

- for the sG potential,

$$\phi(s) = \begin{cases} 2\arccos\left\{cn^2\left[(s - s_0)\pi/d_{\rm kc}, 1/2\right]\right\}, & \text{for } (s > s_0), \\ -2\arccos\left\{cn^2\left[(s - s_0)\pi/d_{\rm kc}, 1/2\right]\right\}, & \text{for } (s < s_0). \end{cases} \tag{12}$$

The static energy of this compacton, following from equation (8) with $v = C_0 = 0$, is given by:

- for the $\phi - four$ potential,

$$E_{\rm kc}^{(0)} = A\omega_0^2 d_{\rm kc}/16. \tag{13}$$

- for the sG potential,

$$E_{\rm kc}^{(0)} = \frac{2^{15/4}}{9\pi^{1/2}}\frac{\Gamma(1/4)}{\Gamma(3/4)}A\omega_0^2 d_{\rm kc}, \tag{14}$$

where $d_{\rm kc}$ may be viewed as the pseudo-kink compacton width, and $cn(x, y)$ and $\Gamma(x)$ are the Jacobi elliptic and the gamma functions, respectively. So the continuum approximation used here is valid only if $d_{\rm kc}/a \gg 1$. Note that, contrary to the kink soliton which has exponentially decreasing wings extending to infinity, the compacton solutions are strictly localized: they have no wings, i.e., they have a compact shape. In the next section, the above expressions will be of particular importance for the determination of different contributions of low-lying excitations including kink solitons and kink compactons on the thermodynamic quantities of the NKG systems.

3. Low-temperature classical statistical mechanics

3.1. Kink soliton systems

The classical partition function for systems governed by the Hamiltonian (1) for the density of states in the phase space is given in the factored form

$$Z = Z_{\dot\phi} Z_\phi, \tag{15}$$

where $Z_{\dot\phi}$ is the kinetic contribution and Z_ϕ the configurational part. The kinetic contribution can be easily evaluated while the configurational part can be evaluated after lengthy algebra by making use of the TIO technique [13], as in the case of the basic NKG models. It yields:

$$Z_{\dot\phi} = \left(2\pi Aa/\beta h^2\right)^{N/2}, \qquad Z_\phi = \sum_{n=0}^{\infty} \exp\left(-\beta A L\omega_0^2 \epsilon_n\right), \tag{16}$$

where $\beta = 1/k_{\rm B}T$, h is Planck's constant and $L = Na$ is the total length of the system of N particles with assumed periodic boundary condition $\phi_{N+1} = \phi_1$. The quantities ϵ_n are the eigenvalues of the TIO defined by

$$\int_{-\infty}^{+\infty} {\rm d}\phi_i \exp\left[-\beta Aa\omega_0^2 f(\phi_{i+1}, \phi_i)\right]\Phi_n(\phi_i) = \exp(-\beta Aa\omega_0^2\epsilon_n)\Phi_n(\phi_{i+1}), \tag{17}$$

where

$$f(\phi_{i+1}, \phi_i) = \frac{C_0^2}{2a^2\omega_0^2}(\phi_{i+1} - \phi_i)^2 + \frac{C_{nl}}{4a^4\omega_0^2}(\phi_{i+1} - \phi_i)^4 + \frac{1}{2}[V_s(\phi_{i+1}) + V_s(\phi_i)]. \quad (18)$$

As pointed out by Trullinger and Sasaki [18], it is possible through a set of transformations and neglecting higher powers in $(a/d_0)^2$ that the transfer integral equation (17), with the first-order lattice corrections included, can be approximated by a Schrödinger-type equation. For the TIO (17) with the function (18), one obtains in a similar way the following Schrödinger equation:

$$-\frac{1}{2m^*}\frac{\mathrm{d}^2\Phi_n(\phi)}{\mathrm{d}\phi^2} + V_{\mathrm{eff}}(\phi)\Phi_n(\phi) = \tilde{\epsilon}_n\Phi_n(\phi), \quad (19)$$

where $\tilde{\epsilon}_n = \epsilon_n - V_0$, with

$$V_0 = -\frac{1}{2\rho}\ln\left[\frac{2\pi a^2}{\rho d_0^2}g_1(y)^2\right], \qquad m^* = [\beta A\omega_0 C_0 g_2(y)]^2, \qquad \rho = \beta A a\omega_0^2, \quad (20)$$

where V_0 is a temperature-dependent energy minimum,

$$g_1(y) = \left(\frac{2y}{\pi}\right)^{1/2}\exp(y)K_{1/4}(y), \quad (21)$$

and

$$g_2(y) = \left\{\frac{K_{1/4}(y)}{4y[K_{3/4}(y) - K_{1/4}(y)]}\right\}^{1/2}. \quad (22)$$

Here, $K_l(y)$ is the modified Bessel function and the parameter y is defined as

$$y = \beta A a C_0^4/8C_{nl}. \quad (23)$$

Equation (19) is the Schrödinger equation for a single particle of mass m^* given by equation (20), and moving in the nonlinear effective potential

$$V_{\mathrm{eff}}(\phi) = V_s(\phi) - \frac{1}{24}\frac{a^2}{d_0^2 g_2(y)^2}\left(\frac{\mathrm{d}V_s(\phi)}{\mathrm{d}\phi}\right)^2, \quad (24)$$

where $g_2(y)$ is given by equation (22). When $C_{nl} = 0 (y \to \infty)$, $g_2(y) = 1$ and the effective potential (24) reduces to that obtained by Trullinger and Sasaki [18] and where d_0 is the mean width of the static kink soliton. In the model under consideration, we can then interpret the quantity

$$d_{\mathrm{eff}} = d_0 g_2(y) \quad (25)$$

as the effective mean width of the static kink in the system where $g_2(y)$ may be viewed as the renormalization coefficient due to the presence of an anharmonic interparticle term [32]. As we will see below, this dependence of the effective kink width on the temperature is at the origin of the dependence, on the temperature, of the first lattice corrections to the thermodynamic properties of the system. Figure (3) shows the variation of the renormalization coefficients $g_1(y)$ and $g_2(y)$ as a function of $1/y$ which is linearly proportional to the interparticle anharmonicity strength and to the temperature. It appears that $g_1(y)$ is a decreasing function of C_{nl} while $g_2(y)$ is an increasing one. The two quantities contain all the information concerning the contribution of the anharmonic interparticle interactions to the thermodynamic quantities of the system.

Note also that equation (18) is identical to the Schrödinger equation obtained for the basic NKG model, except for the fact that the quantities V_0 and m^* depend, here, on the interparticle

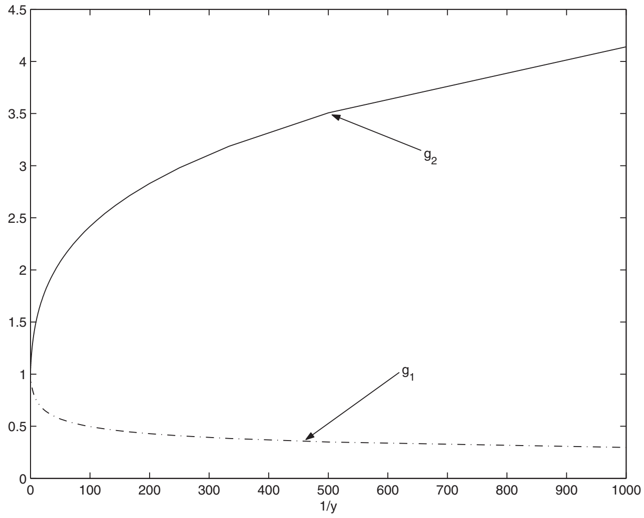

Figure 3. Renormalization coefficients $g_1(y)$ and $g_2(y)$ as a function of $1/y$, where y is given by equation (23).

anharmonicity strength C_{nl} through y. In the limit $C_{nl} \to 0$, i.e., $y \to \infty$, $g_1(y) = 1$ and $g_2(y) = 1$, one recovers the basic results [13, 21]:

$$V_0 = -\frac{1}{2\rho}\ln\left[\frac{2\pi a^2}{\rho d_0^2}\right], \qquad m^* = (\beta A\omega_0 C_0)^2. \tag{26}$$

Accordingly, the Schrödinger equation (18) can be treated by the same technique usually invoked to solve the Schrödinger-type equation obtained for the basic NKG systems. For this purpose, in the thermodynamic limit, ($L \to \infty$, $N \to \infty$ with $L/N = a$ constant), Z_ϕ is dominated by the lowest eigenvalue $\tilde{\epsilon}_0$ and the free-energy per unit length, $f = -(1/\beta L)\ln Z$, becomes

$$f = -\frac{1}{2\beta a}\ln\left(\frac{2\pi Aa}{\beta h^2}\right) + A\omega_0^2 V_0 + A\omega_0^2\tilde{\epsilon}_0. \tag{27}$$

As one can easily see, to evaluate f, the main problem we are faced with consists in the calculation of the lowest eigenvalue $\tilde{\epsilon}_0$ of the Schrödinger operator. In the low-temperature regime $\beta \gg 1 (m^* \gg 1)$, there are several ways to find approximate eigenvalues $\tilde{\epsilon}_0$, all of them known as the improved WKB methods (see [33] and references therein). In the following, we use the procedure developed by Croitoru *et al* (see for example [20, 34]) based on the assumption depending on a large parameter which has the advantage of making a clear distinction between the various contributions to the free energy: phonons, kink, kink–kink interactions, and so on. Following this procedure, the calculation of the ground state, $\tilde{\epsilon}_0$, is similar to the one performed in the case of the basic NKG systems [20, 21]. Then

$$\tilde{\epsilon}_0 = \tilde{\epsilon}_{00}(1 - 2\nu)\left(1 - \frac{1}{24}\frac{a^2}{d_{\text{eff}}^2}\right) \tag{28}$$

for the $\phi - four$ potential, and

$$\tilde{\epsilon}_0 = \tilde{\epsilon}_{00}(1 - 4\nu)\left(1 - \frac{1}{24}\frac{a^2}{d_{\text{eff}}^2}\right) \tag{29}$$

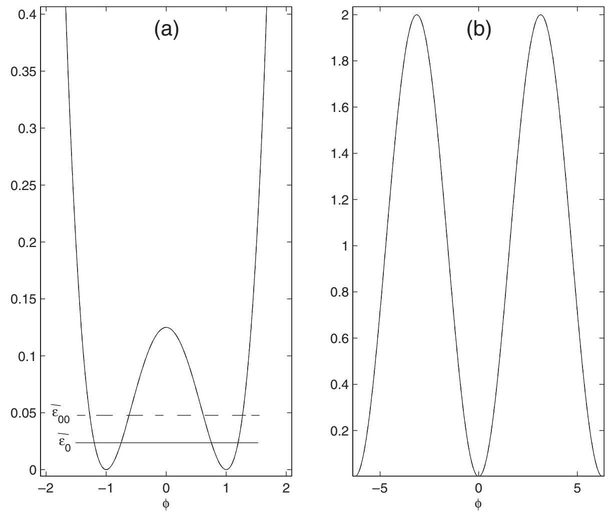

Figure 4. Shape of the effective potential $V_{\text{eff}}(\phi)$ given by equation (24): (a) for the $\phi - four$ potential and (b) for the sG potential. Two cases are considered: $a/d_0 = 0$ (dotted curve), corresponding to the unperturbed substrate potential $V_s(\phi)$, and $a/d_0 = 0.2$ with $g_2(y) = 3.5$, i.e., $1/y = 2 \times 10^{-3}$ (solid curve). The two curves are superposed since they are almost identical. For the $\phi - four$ potential case, the shape of the effective potential is qualitatively different to that of the substrate potential for very large values of ϕ. However, this modification of shape has no effect on the physics of the problem since we are concerned only with the displacement field close to or belonging to the interval $[-1, +1]$ corresponding to phonons and kink like excitations.

for the sG potential, and where $\tilde{\epsilon}_{00}$ is the first term in the asymptotic expansion of the lowest eigenvalue of the isolated potential well given by

$$\tilde{\epsilon}_{00} = 1/(2\sqrt{m^*}). \tag{30}$$

The quantity ν is the small parameter related to the small shift from the eigenvalue of an isolated well due to the presence of the other degenerate minima of the potential represented in figure (4). The presence of these degenerate minima leads to the tunnel splitting of the lowest level $\tilde{\epsilon}_{00}$ of the isolated well. The lower extremity can be found from the boundary conditions for the wavefunction of equation (18) and its derivatives. The result which takes into account the various low-lying excitations contribution is

$$\nu = \nu_k + \nu_{\text{kk}}. \tag{31}$$

The single kink soliton contribution ν_k is given by

$$\nu_k = (6\varpi/\pi)^{1/2}\left(1 - \frac{1}{10}\frac{a^2}{d_{\text{eff}}^2}\right)\exp(-\varpi), \tag{32}$$

with

$$\varpi = \beta E_{\text{eff}}^{(0)}\left(1 - \frac{1}{120}\frac{a^2}{d_{\text{eff}}^2}\right), \qquad E_{\text{eff}}^{(0)} = E_s^{(0)} g_2(y) \tag{33}$$

for the $\phi - four$ potential, and

$$\nu_k = (2\varpi/\pi)^{1/2}\left(1 - \frac{1}{72}\frac{a^2}{d_{\text{eff}}^2}\right)\exp(-\varpi), \tag{34}$$

with

$$\varpi = \beta E_{\rm eff}^{(0)}\left(1 - \frac{1}{72}\frac{a^2}{d_{\rm eff}^2}\right), \qquad E_{\rm eff}^{(0)} = E_s^{(0)} g_2(y) \tag{35}$$

for the sG potential, where $E_s^{(0)}$ is the well-known static kink soliton energy of the basic NKG systems defined in equation (9) and equation (10) for the $\phi - four$ and for the sG potentials, respectively. The quantity $E_{\rm eff}^{(0)}$ may be viewed as the renormalized static kink energy in the system, due to the anharmonicity of the interparticle interactions [32]. The quantity $\nu_{\rm kk}$ is the contribution of kink–kink interactions and is given by

$$\nu_{\rm kk} = -\nu_k^2\left[\ln(12\gamma\varpi) - \frac{1}{5}\frac{a^2}{d_{\rm eff}^2}\right] \tag{36}$$

for the $\phi - four$ potential, and

$$\nu_{\rm kk} = -2\nu_k^2\left[\ln(4\gamma\varpi) - \frac{1}{36}\frac{a^2}{d_{\rm eff}^2}\right] \tag{37}$$

for the sG potential, with $\gamma = 1.781\,072\ldots$, the Euler constant. The imaginary part of $\nu_{\rm kk}$, $\pi\nu_k^2$ for the sG and for the $\phi - four$ potentials, is omitted in the above expression and is out of scope of the paper. Nevertheless, it can be interpreted as a quantity describing the finite lifetime of each state of the potential [21]. In the limit of vanishing C_{nl}, this result is in complete agreement with that found by Grecu and Visinescu [20]. We are now in possession of the relevant parameter, $\tilde{\epsilon}_0$, entering in the construction of the thermodynamic properties of the system:

$$\begin{aligned}\tilde{\epsilon}_0 = {}& \frac{1}{2\sqrt{m^*}}\left(1 - \frac{1}{24}\frac{a^2}{d_{\rm eff}^2}\right) - \frac{1}{\sqrt{m^*}}\left(1 - \frac{17}{120}\frac{a^2}{d_{\rm eff}^2}\right)\\ & \times (6\varpi/\pi)^{1/2}\exp(-\varpi)\left\{1 - \nu_k\left[\ln(12\gamma\varpi) - \frac{1}{5}\frac{a^2}{d_{\rm eff}^2}\right]\right\}\end{aligned} \tag{38}$$

for the $\phi - four$ potential, and

$$\begin{aligned}\tilde{\epsilon}_0 = {}& \frac{1}{2\sqrt{m^*}}\left(1 - \frac{1}{24}\frac{a^2}{d_{\rm eff}^2}\right) - \frac{2}{\sqrt{m^*}}\left(1 - \frac{1}{18}\frac{a^2}{d_{\rm eff}^2}\right)\\ & \times (2\varpi/\pi)^{1/2}\exp(-\varpi)\left\{1 - 2\nu_k\left[\ln(4\gamma\varpi) - \frac{1}{36}\frac{a^2}{d_{\rm eff}^2}\right]\right\}\end{aligned} \tag{39}$$

for the sG potential. The interparticle anharmonicity strength C_{nl} enters in the above expressions through the effective mass m^*.

Based on the treatment of the basic NKG systems, we can then separate the free-energy into two parts: $f = f_{\rm ph} + f_{\rm tun}$; the phonon part is $f_{\rm ph}$, and the tunnelling or soliton part is $f_{\rm tun}$. The first part is given by

$$f_{\rm ph} = \frac{1}{\beta a}\ln\left(\frac{\beta\hbar C_0}{a g_1(y)}\right) + \frac{1}{2\beta d_{\rm eff}}\left(1 - \frac{1}{24}\frac{a^2}{d_{\rm eff}^2}\right), \tag{40}$$

both for the $\phi - four$ and the sG potentials. The second part, which is the tunnelling contribution written in the form known from the soliton kink gas approach [16, 17, 21] and which evidences the contribution of kink compaction–kink compaction interactions, is given by

$$f_{\rm tun} = -k_{\rm B}T n_k^{(c)}\left(1 - B_k^{(c)} n_k^{(c)}\right), \tag{41}$$

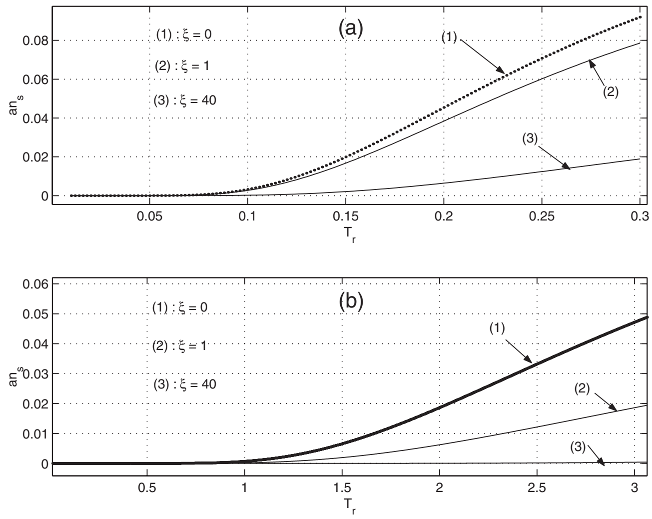

Figure 5. Kink soliton density $n_k^{(c)}$ as a function of the reduced temperature $T_r = k_B T/A\omega_0 C_0$ and for three values of the dimensionless interparticle anharmonicity strength $\xi = C_{nl}/C_0^2$: (a) for the $\phi - four$ potential and (b) for the sG potential.

with

$$n_k^{(c)} = \frac{1}{d_{\text{eff}}}\left(\frac{6\beta E_{\text{eff}}^{(c)}}{\pi}\right)^{1/2}\left(1 - \frac{17}{120}\frac{a^2}{d_{\text{eff}}^2}\right)\exp\left[-\beta E_{\text{eff}}^{(c)}\right] \tag{42}$$

and

$$B_k^{(c)} = d_{\text{eff}}\left(1 + \frac{1}{24}\frac{a^2}{d_{\text{eff}}^2}\right)\left[\ln(12\gamma\beta E_{\text{eff}}^{(c)}) - \frac{1}{5}\frac{a^2}{d_{\text{eff}}^2}\right] \tag{43}$$

for the $\phi - four$ potential, and

$$n_k^{(c)} = \frac{2}{d_{\text{eff}}}\left(\frac{2\beta E_{\text{eff}}^{(c)}}{\pi}\right)^{1/2}\left(1 - \frac{1}{18}\frac{a^2}{d_{\text{eff}}^2}\right)\exp[-\beta E_{\text{eff}}^{(c)}], \tag{44}$$

and

$$B_k^{(c)} = d_{\text{eff}}\left(1 + \frac{1}{24}\frac{a^2}{d_{\text{eff}}^2}\right)\left[\ln(4\gamma\beta E_{\text{eff}}^{(c)}) - \frac{1}{36}\frac{a^2}{d_{\text{eff}}^2}\right], \tag{45}$$

for the sG potential. Equations (41)–(43) are, in the limit $(a/d_0)^2 \to 0$, in complete agreement with previous calculations of the kink soliton and kink soliton–kink soliton sector contributions [32]. Similarly, in the limit $C_{nl} = 0$, they are also in complete agreement with the results of the kink and kink–kink contributions for the basic NKG systems [20]. Therefore, the quantity $n_k^{(c)}$, plotted in figure (5), can be identified as the kink soliton density within the ideal gas soliton approach while the quantity $B_k^{(c)}$ may be viewed as the second virial coefficient resulting from the soliton–soliton interactions. These quantities are corrected by the lattice effects.

As is seen from equations (41)–(45), in the kink soliton contribution there appears a lattice corrected kink energy

$$E_{\text{eff}}^{(c)} = E_{\text{eff}}^{(0)}\left(1 - \frac{1}{120}\frac{a^2}{d_{\text{eff}}^2}\right) \tag{46}$$

for the $\phi - four$ potential, and

$$E_{\rm eff}^{(c)} = E_{\rm eff}^{(0)}\left(1 - \frac{1}{72}\frac{a^2}{d_{\rm eff}^2}\right) \tag{47}$$

for the sG potential, where $E_{\rm eff}^{(0)}$ is the known unperturbed kink soliton energy defined by equation (33) and by (35) for the $\phi - four$ and the sG potentials, respectively. It appears that $E_{\rm eff}^{(0)}$ is temperature dependent and is different from the static kink soliton energy calculated in section 2 (see equations (6) and (7)). Thus, one may view $E_{\rm eff}^{(0)}$ as the effective energy of the static kink soliton which takes into account the nonlinear interaction between kink solitons and phonons, induced by the anharmonicity of the interparticle interaction. Similarly, the correction factor appearing in the lattice corrected expressions of the energy, equations (46) and (47), and those appearing in the expression of the free-energy, due to lattice effects, are temperature dependent since the effective mean width of the kink in the system, $d_{\rm eff}$, depends on the temperature. This dependence results in the anharmonic interactions or inelastic collision between low-lying excitations due to the anharmonicity of the interparticle interactions. The above results suggest that, in the system where the interactions between particles are anharmonic, the first lattice corrections are temperature dependent and become less and less important when the temperature is increased.

3.2. Purely anharmonic case: kink compacton systems

The classical partition function for systems governed by the Hamiltonian (1), with $C_0 = 0$, for the density of states in the phase space is given in factored form by equation (15), where the kinetic contribution $Z_{\dot\phi}$ and the configurational part Z_ϕ are given by equation (16) with ϵ_n the eigenvalues of the TIO defined by equation (17). In this case, the corresponding TIO can be approximated in a similar way through a set of transformations and neglecting higher powers in $(a/d_{\rm kc})^2$, i.e., including the first lattice corrections, by the same Schrödinger equation (19) for the eigenfunction Φ_n:

$$-\frac{1}{2m'^*}\frac{{\rm d}^2\Phi_n(\phi)}{{\rm d}\phi^2} + V_{\rm eff}(\phi)\Phi_n(\phi) = \tilde\epsilon_n\Phi_n(\phi), \tag{48}$$

where $\tilde\epsilon_n = \epsilon_n - V_0'$. However, the temperature-dependent energy minimum V_0' and the parameter m'^* are now given by

$$\begin{aligned} m'^* &= \beta Aa\omega_0^2\left(\frac{\beta AC_{nl}}{4a^3}\right)^{1/2}\frac{\Gamma(1/4)}{\Gamma(3/4)}, \\ V_0' &= -\frac{1}{\beta Aa\omega_0^2}\ln\left[\frac{\sqrt{2}\Gamma(1/4)^2}{4}\left(\frac{a^3}{\beta AC_{nl}}\right)^{1/2}\right]. \end{aligned} \tag{49}$$

Similarly, the effective potential is also rewritten as follows:

$$V_{\rm eff}(\phi) = V_s(\phi) - \Lambda\left(\frac{{\rm d}V_s(\phi)}{{\rm d}\phi}\right)^2, \tag{50}$$

with

$$\Lambda = \frac{\pi^2}{(24\eta)^{1/2}}\frac{\Gamma(3/4)}{\Gamma(1/4)}\left(\frac{a}{d_{\rm kc}}\right)^2\left(\beta Aa\omega_0^2\right)^{1/2}, \tag{51}$$

where η is the model-dependent numerical coefficient defined in section 2. As is seen from equation (51), the effective potential depends on the temperature through the discreteness coefficient Λ, and then this dependence is at the origin of the dependence, on the temperature, of the fist lattice corrections to the thermodynamic properties of the system. As in the case of kink soliton systems of the preceding subsection, in the thermodynamic limit ($L \to \infty$, $N \to \infty$ with $L/N = a$ constant), Z_ϕ is dominated by the lowest eigenvalue $\tilde{\epsilon}'_0$ and the free-energy per unit length, f, becomes

$$f = \frac{1}{4\beta a} \ln \left[\frac{4\beta^3 h^4 C_{nl}}{\pi^2 \Gamma(1/4)^4 A a^5} \right] + A\omega_0^2 \tilde{\epsilon}'_0, \tag{52}$$

where $\tilde{\epsilon}'_0 \equiv \epsilon_{n=0}$.

By making use of the procedure of the preceding subsection for solving $\tilde{\epsilon}'_0$, the lowest eigenvalue $\tilde{\epsilon}'_0$ of the Schrödinger equation (48) is then given by

$$\tilde{\epsilon}'_0 = \tilde{\epsilon}'_{00}(1 - 2\nu_c)(1 - \Lambda) \tag{53}$$

for the $\phi - four$ potential, and

$$\tilde{\epsilon}'_0 = \tilde{\epsilon}'_{00}(1 - 4\nu_c)(1 - \Lambda) \tag{54}$$

for the sG potential, and where $\tilde{\epsilon}'_{00}$ is the first term in the asymptotic expansion of the lowest eigenvalue of the isolated potential well, given by

$$\tilde{\epsilon}'_{00} = 1/2\sqrt{m'^*}. \tag{55}$$

The quantity ν_c is a small parameter related to the small shift from the eigenvalue of an isolated well due to the presence of the other degenerate minima of the potential. It can also be separated into two parts, the single kink compacton contribution ν_{kc} and the kink compacton–kink compacton interactions contribution ν_{kckc}:

$$\nu_{\mathrm{c}} = \nu_{\mathrm{kc}} + \nu_{\mathrm{kckc}}. \tag{56}$$

The analytical expressions of these contributions are given by

$$\nu_{\mathrm{kc}} = (6\varpi_{\mathrm{c}}/\pi)^{1/2}(1 - \tfrac{24}{10}\Lambda)\exp(-\varpi_{\mathrm{c}}), \tag{57}$$

$$\nu_{\mathrm{kckc}} = -\nu_{\mathrm{kc}}^2[\ln(12\gamma\varpi_{\mathrm{c}}) - \tfrac{24}{5}\Lambda] \tag{58}$$

with

$$\varpi_{\mathrm{c}} = \chi[\beta E_{\mathrm{kc}}^{(0)}(1 - \tfrac{4}{15}\Lambda)]^{3/4}, \qquad \chi = \frac{1}{\pi}\left(\frac{2^{13}}{3^5}\right)^{1/4}\left[\frac{\Gamma(1/4)}{\Gamma(3/4)}\right]^{1/2}\left(\frac{d_{\mathrm{kc}}}{a}\right)^{1/4} \tag{59}$$

for the $\phi - four$ potential, and

$$\nu_{\mathrm{kc}} = (2\varpi_{\mathrm{c}}/\pi)^{1/2}(1 - \tfrac{1}{3}\Lambda)\exp(-\varpi_{\mathrm{c}}), \tag{60}$$

$$\nu_{\mathrm{kckc}} = -2\nu_{\mathrm{kc}}^2[\ln(4\gamma\varpi) - \tfrac{2}{3}\Lambda] \tag{61}$$

with

$$\varpi_{\mathrm{c}} = \chi[\beta E_{\mathrm{kc}}^{(0)}(1 - \tfrac{4}{9}\Lambda)]^{3/4}, \qquad \chi = \left[\frac{3^5 2^{3/4}}{\pi^{5/2}}\frac{\Gamma(3/4)}{\Gamma(1/4)}\frac{d_{\mathrm{kc}}}{a}\right]^{1/4} \tag{62}$$

for the sG potential. The quantity $E_{\mathrm{kc}}^{(0)}$ is the static kink compacton energy defined in the preceding section. By inserting the above expressions of ν_{kc} and ν_{kckc} in (56), we then obtain the lowest eigenvalue $\tilde{\epsilon}'_0$. Since we are in possession of the lowest eigenvalue, the free-energy which follows from equation (52) can be separated into two parts: $f = f_{\mathrm{aph}} + f_{\mathrm{tun}}$. The first part f_{aph}, which may be viewed as the contribution of anharmonic phonons, is given for both potentials by

$$f_{\mathrm{aph}} = \frac{1}{4\beta a}\ln\left[\frac{4\beta^3 h^4 C_{nl}}{\pi^2\Gamma(1/4)^4 A a^5}\right] + \frac{\pi}{2}\left(\frac{24}{\eta}\right)^{1/4}\left[\frac{\Gamma(3/4)}{\Gamma(1/4)}\right]^{1/2}\frac{\left(Aa\omega_0^2\right)^{1/4}}{\beta^{3/4} d_{\mathrm{kc}}}(1 - \Lambda). \tag{63}$$

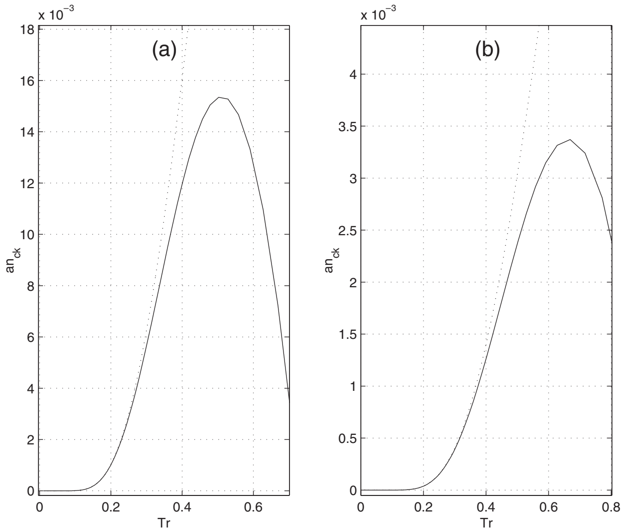

Figure 6. Kink compacton density as a function of the reduced temperature $T_r = k_B T/E_{kc}^{(0)}$: (a) for the $\phi - four$ potential, and (b) for the sG potential. The dotted line represents the curve of the quantity $n_{kc}^{(c)}$ while the solid line is the curve of the quantity $n_{kc} = n_{kc}^{(c)}[1 - 2B_{kc}^{(c)} n_{kc}^{(c)}]$ designating the density of kink compactons which takes into account the interactions between kink compactons.

The tunnelling part or the contribution of kink compactons f_{tun} is also given by

$$f_{tun} = -k_B T n_{kc}^{(c)}[1 - B_{kc}^{(c)} n_{kc}^{(c)}], \tag{64}$$

with

$$n_{kc}^{(c)} = \left(\frac{2^{11}}{3\pi}\right)^{1/2} \frac{(\beta E_{kc}^{(c)})^{5/8}}{d_{kc}\chi^{1/2}} \left(1 - \frac{10}{3}\Lambda\right) \exp[-\chi(\beta E_{kc}^{(c)})^{3/4}], \tag{65}$$

$$B_{kc}^{(c)} = \tfrac{3}{32}\chi(\beta E_{kc}^{(c)})^{-1/4} d_{kc}(1 + \tfrac{14}{15}\Lambda)\{\ln[12\gamma\chi(\beta E_{kc}^{(c)})^{3/4}] - \tfrac{24}{5}\Lambda\} \tag{66}$$

for the $\phi - four$ potential, and

$$n_{kc}^{(c)} = 9 \times 2^{3/4} \frac{\Gamma(3/4)}{\Gamma(1/4)} \frac{(\beta E_{kc}^{(c)})^{5/8}}{d_{kc}\chi^{1/2}} \left(1 - \frac{11}{9}\Lambda\right) \exp[-\chi(\beta E_{kc}^{(c)})^{3/4}], \tag{67}$$

and

$$B_{kc}^{(c)} = \frac{2^{3/4}}{9\sqrt{\pi}} \frac{\Gamma(1/4)}{\Gamma(3/4)} \chi(\beta E_{kc}^{(c)})^{-1/4} d_{kc} \left(1 + \frac{14}{15}\Lambda\right) \left\{\ln[4\gamma\chi(\beta E_{kc}^{(c)})^{3/4}] - \frac{2}{3}\Lambda\right\} \tag{68}$$

for the sG potential. $n_{kc}^{(c)}$, plotted in figure 6, may be viewed as the lattice corrected kink compacton density within the ideal gas limit while $B_{kc}^{(c)}$ represents the second virial coefficient. In the limit $(a/d_{kc})^2 \to 0$, the above results, equations (56)–(68), reduce to the previous results of kink compacton contribution to the free-energy [32].

As is seen from equations (59) and (62), in the kink compacton or tunnelling contribution there appears a lattice corrected kink compacton energy

$$E_{kc}^{(c)} = E_{kc}^{(0)}(1 - \tfrac{4}{15}\Lambda) \tag{69}$$

for the $\phi - four$ potential, and

$$E_{kc}^{(c)} = E_{kc}^{(0)}(1 - \tfrac{4}{9}\Lambda) \tag{70}$$

for the sG potential, where $E_{kc}^{(0)}$ is the known unperturbed static kink compacton energy defined by equations (13) and (14) for the $\phi - four$ and the sG potentials, respectively. It is obvious that the correction factor of this energy and those appearing in the expression of the free-energy due to lattice effects are temperature dependent, since the discreteness coefficient Λ depends on the temperature. The above temperature dependence of the lattice corrected kink compacton energy may be attributed to nonlinear interactions between kink and lattice anharmonic phonons.

4. Conclusion

In this paper, we have investigated the low-temperature classical statistical mechanics of discrete nonlinear Klein–Gordon (NKG) systems with anharmonic interparticle interactions which takes into account the lattice corrections due to the discrete character of the systems. In addition, our study has taken into account the two kink interactions in the system. Thus, we have used the transfer integral operator (TIO) with the first lattice corrections included by considering terms of order $(a/d_0)^2$ where d_0 is the mean width of the kink solitons and a the lattice constant. Two particular substrate potentials have been considered: the $\phi - four$ and the sine-Gordon (sG) potentials.

We have first focused our attention on the case where the system may exhibit the static kink soliton as a solution of the resulting generalized NKG equation. The obtained results reveal a dependence of the first lattice corrections to the free-energy in particular, and consequently to other thermodynamic quantities in general, to the temperature. This dependence of the first lattice corrections to thermodynamic properties of the system results from the fact that the first lattice corrections are a function of the effective width of kink solitons which, in the NKG models with anharmonic interparticle interactions, depends on the temperature through a coupling between the interparticle anharmonicity strength and the temperature. Furthermore, these results show also that the increase of the temperature lowers the discreetness effects and the correction terms in the thermodynamic quantities become less and less important as the temperature is increased.

Next, we have considered the limiting case of the purely anharmonic NKG systems for which the stable static kink compacton like excitations can be obtained. Here, the thermodynamic quantities such as the free-energy are sensitive to this kind of excitation. We have shown that the first lattice corrections to the free-energy of the system and to the static kink compacton rest energy are also temperature dependent. Futhermore, the discreteness coefficient due to lattice discreteness is proportional to $\sim(a/d_{kc})^2 T^{-1/2}$, i.e., is a function of the kink compacton mean width. The analysis of these results shows that the lattice effects decrease for increasing temperatures as in the case of the NKG systems with anharmonic interparticle interactions exhibiting kink solitons.

Finally, we mention that such temperature dependence of discreteness effects to the classical statistical mechanics of kink gas has been already obtained in the case of the basic NKG systems. However, and contrary to our results where even the first lattice corrections are temperature dependent, the temperature enters in their results through the pinning potential barriers, i.e., when the system is highly discrete and then where the trapping of kinks is more important compared to the first lattice corrections which are independent of the temperature. Note that our results are valid for a weakly discrete system and where the kink width is greater than the lattice spacing. In this limit, the first lattice corrections are more important compared to the contribution of the pinning potential.

As previously mentioned [32], it is important to note also that, although a proof of a similar CKBT phenomenology does not exist at present, we think that the temperature dependence of the first lattice corrections to the thermodynamic properties of the system may be attributed to nonlinear interactions between the different low-lying excitations of the system induced by the anharmonicity of the interparticle interactions. It should then be interesting to establish a proof similar to the CKBT phenomenology which takes into account the renormalization of kink soliton parameters due to the anharmonicity of the interparticle interactions. This problem is already under consideration.

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