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Kink compactons in the thermodynamic properties of nonlinear Klein–Gordon systems

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Abstract

Thermodynamic properties of one-dimensional nonlinear Klein–Gordon systems with anharmonic interparticle interaction are studied by means of the transfer integral method. We show that the presence of kink compactons is signalled by a term proportional to $\exp[-\chi(\beta E_{\mathrm{kc}})^{3/4}]$ in the free energy where E_{kc} is the static kink compacton energy and χ a model temperature independent coefficient.

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1. Introduction

Many nonlinear physical systems that exhibit the propagation of large amplitude excitations such as solitons, have been the subject of considerable interest for many decades. These solitons are the result of interplay between the nonlinear and dispersive effects. Condensed matter systems have been more solicited. This particular attention is justified by the role played by kink solitons in many areas of condensed matter, since they have been used to describe various phenomena such as dislocation in crystals [1], planar domain walls in ferromagnets [2], incommensurate systems [3], proton motion in hydrogen-bonded systems ranging from ferroelectrics to biomolecules [4–6], to name only a few. Many of them are modelled by the well-known nonlinear Klein–Gordon (NKG) models where the lattice models consist of harmonically coupled particles subjected to an on-site substrate potential, which possesses more than one degenerate minima. This spatial degeneracy, associated with the harmonic coupling between lattice sites, provides kink solitons with infinite wings, which cause mutual interactions. The thermodynamics at low temperature of such systems is well known. It has been shown, through the transfer integral operator (TIO) method [4, 7, 9, 10] and the kink-gas phenomenology [8, 9, 11], that the low-temperature thermodynamics of the system is sensitive to and even dominated by static kink solitons; their presence in the system is signalled by a term proportional to $\exp(-E_{\mathrm{k}}/k_{\mathrm{B}}T)$ in the low-temperature free energy, where E_{k} is the *static kink energy*.

However, as demonstrated by Rosenau and Hyman [12], who investigated a special type of Korteweg–de-Vries equation, another kind of soliton excitation without infinite tail can be obtained. These solitary waves with compact support are called compactons and result in nonlinear dispersion which is capable of causing deep qualitative changes in the nature of genuinely nonlinear phenomena. Similarly, Kivshar has pointed out that intrinsic localized modes in purely anharmonic lattices may exhibit compacton-like properties [13]. Recently, Dusuel *et al* [14] demonstrated theoretically and experimentally with the nonlinear coupled pendulum that kink compacton excitations can appear in NKG models. This work was later improved by Maximo *et al* [15] who evidenced another kind of compacton in the system such as drop compactons (soliton with compact support in the shape of hard spheres), cups, peak solitons or peakons and defects. Very recently, using the method of constructing exact solutions on lattices proposed by Kinnersley and described in [16], Kevrekidis *et al* [17] have calculated the exact compacton solutions in a discrete system and have examined the linear stability of such solutions, for the bright and the dark compactons, respectively.

As condensed matter systems are one of the physical systems whose dynamics can be satisfactorily described by the generalized NKG models and where the number of low-lying excitations is thermally controlled, the effect of kink compactons on the thermodynamic properties of kink compacton-bearing systems is still an open question, although since the pioneering work of Rosenau and Hyman [12] much progress have been made in order to understand the dynamical properties of these systems. To cite just two examples, we mention that the ability of kink compactons to execute a stable ballistic propagation in discrete NKG systems with anharmonic coupling [18] and the existence of breather compactons [19] have been investigated. In other words*, does the presence of kink compactons still remain signalled by terms proportional to* $\exp(-E_{\mathrm{k}}/k_{\mathrm{B}}T)$ *in the thermodynamic quantities of the systems exhibiting kink compactons as is the case of kink solitons of basic NKG models*? We try to answer the above stated question, since up to now there are no investigations of this issue, and this is the main objective of this paper. Before continuing, we would like to mention that the inclusion of anharmonic forces or interactions is generally dictated by some experimental results. In this spirit, some previous models [20] have indicated that the inclusion of anharmonic forces can give an answer to the problem of heat conduction in one-dimensional (1D) insulating solids. In addition, it has been demonstrated that for sufficiently high energies/temperatures where the usual picture of weakly interacting phonons is no longer appropriate, one has to face a fully nonlinear problem and a complete analytical solution seems hardly feasible [20].

The organization of the paper is as follows: in section 2, we present the Hamiltonian model of the generalized NKG systems and discuss qualitatively the existence of low-energy excitations (phonons, kink solitons and kink compactons) of the resulting equation of motion for the field. In section 3, we use the TIO method [4] to approximate the partition function into an equivalent Schrödinger-type equation. Using asymptotic methods from the theory of differential equations depending on a large parameter, to solve this equation, the contributions of low-energy excitations to the free energy are then obtained. Section 4 gives concluding remarks.

2. Model, kink soliton and kink compacton-like excitations

To begin, we consider a system of particles of mass m anharmonically coupled to their nearest neighbours and placed on an infinite 1D lattice of spacing a. The Hamiltonian of this discrete chain may be written as

$$H = Aa \sum \left\{ \frac{1}{2} \left(\frac{\mathrm{d}\phi_i}{\mathrm{d}t} \right)^2 + U(\phi_{i+1} - \phi_i) + \omega_0^2 V_{\mathrm{s}}(\phi) \right\}, \tag{2.1}$$

with the interatomic interaction pair potential $U(\phi_{i+1} - \phi_i)$ taken as

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

where ϕ_i denotes the dimensionless displacement of the ith particle measured from the ith lattice site. The constant C_0 is a characteristic velocity, ω_0 is a characteristic frequency, $d_0 = C_0/\omega_0$ defines the characteristic length scale of the basic NKG systems and the factor $A \approx ma$ sets the energy scale of the system. The parameter C_{nl} controls the strength of the nonlinear interparticle coupling.

The last term of equation (2.1), $V_{\mathrm{s}}(\phi)$, is the on-site or substrate potential and has at least two degenerate minima. Here, we consider two specific substrate potentials: the ϕ-four potential $V_{\mathrm{s}}(\phi) = \frac{1}{8}(1 - \phi^2)^2$ and the sine-Gordon (sG) potential $V_{\mathrm{s}}(\phi) = 1 - \cos(\phi)$. When $C_{\mathrm{nl}} = 0$, the Hamiltonian (2.1) reduces to the basic NKG systems Hamiltonian in the notation of Currie, Krumhansl, Bishop and Trullinger (CKBT) [9].

In the continuum or 'displacive' limit, the Hamiltonian (2.1) is transformed approximately to

$$H = Aa \int \frac{\mathrm{d}x}{a} \left[\frac{1}{2} \left(\frac{\partial \phi}{\partial t} \right)^2 + \frac{1}{2} C_0^2 \left(\frac{\partial \phi}{\partial x} \right)^2 + \frac{1}{4} C_{\mathrm{nl}} \left(\frac{\partial \phi}{\partial x} \right)^4 + \omega_0^2 V_{\mathrm{s}}(\phi) \right]. \tag{2.3}$$

We shall have the occasion to use both forms ((2.1) and (2.3)) 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 (2.3) is used to study qualitatively the behaviour of the system. The excitations of the system arise as solutions to the Euler–Lagrange equation of motion following from equation (2.3):

$$\phi_{tt} - C_0^2 \phi_{xx} - 3C_{\mathrm{nl}} \phi_x^2 \phi_{xx} + \omega_0^2 \, \mathrm{d}V_{\mathrm{s}}(\phi)/\mathrm{d}\phi = 0, \tag{2.4}$$

where the subscripts indicate partial derivatives with respect to time t and space $x = \mathrm{i}a$. We look for travelling waves of the form $\phi = \phi(s) = \phi(x - vt)$ where s is a single independent variable depending on v which is an arbitrary velocity of propagation. The first integral resulting from equation (2.4) is then given by

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}s} \right)^4 - \frac{2\left(v^2 - C_0^2\right)}{3C_{\mathrm{nl}}} \left(\frac{\mathrm{d}\phi}{\mathrm{d}s} \right)^2 - \frac{4\omega_0^2}{3C_{\mathrm{nl}}} [V_{\mathrm{s}}(\phi) + C_1] = 0, \tag{2.5}$$

where C_1 is an integration constant.

Depending on the magnitude and on the sign of the nonlinear coupling C_{nl}, the nonlinear partial differential equation (2.4) may sustain different kinds of nonlinear excitations. For the basic NKG systems obtained by setting $C_{\mathrm{nl}} = 0$, the phase plane $(\phi, p = \mathrm{d}\phi/\mathrm{d}s)$ resulting from equation (2.4) is well known: the equilibrium solutions are $\phi(s) = 0$, -1 and $+1$ for the ϕ-four potential and $\phi(s) = 0, \pi$ and 2π in one period for the sG potential. The kink solitons are trajectories connecting $(\phi, p) = (-1, 0)$ and $(+1, 0)$ for the ϕ-four potential

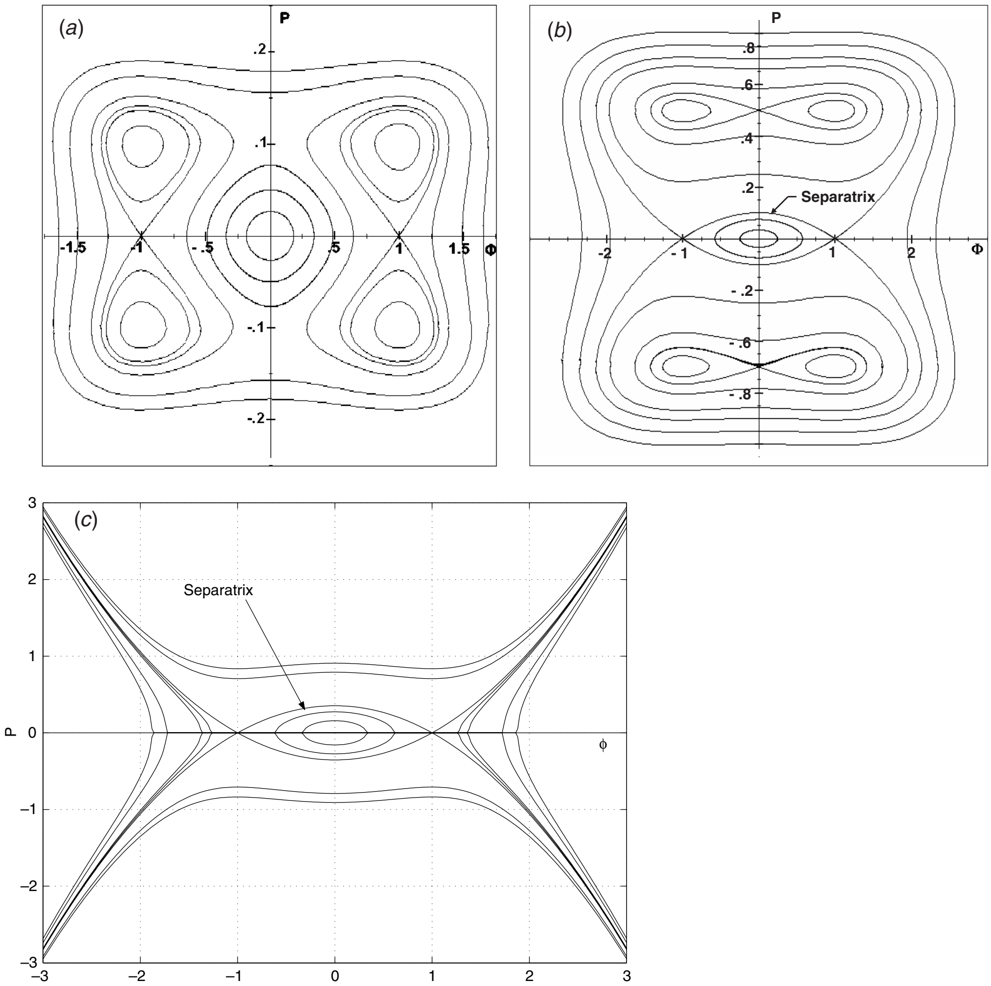

Figure 1. An example of the phase trajectories of the system governed by equation (2.4), $p(\phi) = \mathrm{d}\phi/\mathrm{d}s$ as a function of ϕ: the ϕ-four potential case. The values of the characteristic parameters of the system are $\omega_0/C_0 = 0.2$ and (*a*) $C_{\mathrm{nl}}/C_0^2 = -100/3 < C_{\mathrm{nl}}^{\mathrm{th}}/C_0^2$, note the absence of the separatrix due to the fact that $C_{\mathrm{nl}} < C_{\mathrm{nl}}^{\mathrm{th}}$, (*b*) $C_{\mathrm{nl}}/C_0^2 = -4/3 > C_{\mathrm{nl}}^{\mathrm{th}}/C_0^2$ and (*c*) $C_{\mathrm{nl}}/C_0^2 = 4/3 > C_{\mathrm{nl}}^{\mathrm{th}}/C_0^2$.

and $(\phi, p) = (0, 0)$ and $(2\pi, 0)$ for the sG potential. These trajectories are known as the separatrices and are obtained by taking the constant $C_1 = 0$ in equation (2.5).

When $C_{\mathrm{nl}} < 0$ and in the low-velocity regime, the phase plane exhibits the same kind of trajectories as for the basic NKG models (see figure 1(*a*)). In addition, a few more singular points $(\phi, p) = (\pm 1, \pm p_0)$ with $p_0 = \left[\left(v^2 - C_0^2\right)/3C_{\mathrm{nl}}\right]^{1/2}$ for the ϕ-four potential and $(\phi, p) = (0, \pm p_0)$ and $(2\pi, \pm p_0)$ for the sG potential, and two more families of closed phase trajectories appear, indicating the presence of new types of solutions which are not known in the basic NKG systems. On the other hand, the presence of the separatrix is subject to the condition

$$\left(v^2 - C_0^2\right)^2 > -3\omega_0^2\eta C_{\mathrm{nl}}, \tag{2.6}$$

where η is the model-dependent numerical coefficient: $\eta = 1$ for the ϕ-four potential and $\eta = 8$ for the sG potential (see figure 1(*b*)) . This means that the existence and the propagation of kink solitons in the system are possible only in the case of weakly nonlinear interparticle coupling $\left(C_{\rm nl} > C_{\rm nl}^{\rm th} = -C_0^4/3\eta\omega_0^2\right)$. Thus, within this condition the kink soliton velocity must be lower than the threshold value $v_{\rm th} = \left(C_0^2 - \omega_0\sqrt{-3\eta C_{\rm nl}/2}\right)^{1/2}$.

When $C_{\rm nl} > 0$, the phase plane of the system in the low-velocity regime, as plotted in figure 1(*c*), and that of the basic NKG systems are qualitatively equivalent. As previously mentioned [14], the kink soliton has a compact structure when $v = C_0$ and more interestingly, in the purely anharmonic case ($C_0 = 0$), the system exhibits a stable static kink compacton. This compacton kink is signalled in the phase plane by the separatrix. Its expression, $\phi_{\rm kc}(s)$, following from equation (2.5) with $C_1 = 0$ and $v = C_0 = 0$, and its corresponding energy $E_{\rm kc}$ are given by [14]:

$$\phi_{\rm kc}(s) = \pm\sin[(s - s_0)/\gamma], \qquad E_{\rm kc} = A\omega_0^2 d_{\rm kc}/16, \tag{2.7}$$

with $|s - s_0| < d_{\rm kc}/2$, for the ϕ-four potential, and

$$\begin{aligned} \phi_{\rm kc}(s) &= 2\arccos\{{\rm cn}^2[(s - s_0)/\gamma, 1/2]\} \qquad \text{for} \quad s \geqslant s_0, \\ \phi_{\rm kc}(s) &= -2\arccos\{{\rm cn}^2[(s - s_0)/\gamma, 1/2]\} \qquad \text{for} \quad s \leqslant s_0, \end{aligned} \tag{2.8a}$$

$$E_{\rm kc} = \frac{2^{15/4}}{9\sqrt{\pi}}\frac{\Gamma(1/4)}{\Gamma(3/4)}A\omega_0^2 d_{\rm kc}, \tag{2.8b}$$

for the sG potential. The quantities γ and $d_{\rm kc}$ are given by

$$\gamma = \left(6C_{\rm nl}/\eta\omega_0^2\right)^{1/4} \qquad \text{and} \qquad d_{\rm ck} = \pi\gamma, \tag{2.9}$$

and designate the characteristic length scale of the purely anharmonic system and the width of the kink compacton, respectively. The functions cn(x, y) and $\Gamma(x)$ are the Jacobi elliptic function and the Gamma function, respectively. So, the continuum approximation used here is valid only if $d_{\rm kc}/a \gg 1$. In contrast to the kink soliton which has exponentially decreasing wings extending to infinity, solutions (2.7) and (2.8*a*) are strictly localized: they have no wings, that is, they have a compact shape (see figure 2). Such solutions occur because in (2.5) the nonlinear coupling term, which corresponds to nonlinear dispersion, is preponderant: the linear coupling term can be zero. In the next section, we shall confine our attention to the case of positive $C_{\rm nl}$ since in this case, the low-temperature statistical mechanics of the system could be influenced by static kink compactons.

3. Low-temperature statistical mechanics

The classical partition function for systems governed by the Hamiltonian (2.1) for density of states in the phase space is given in the factored form $Z = Z_{\dot\phi}Z_\phi$, 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 [4] as in the case of the basic NKG systems. One obtains

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

where $\beta = 1/k_{\rm B}T$, $k_{\rm B}$ being the Boltzmann constant, T the absolute temperature, h the Planck constant and $L = Na$ the total length of the chain of N particles with assumed periodic

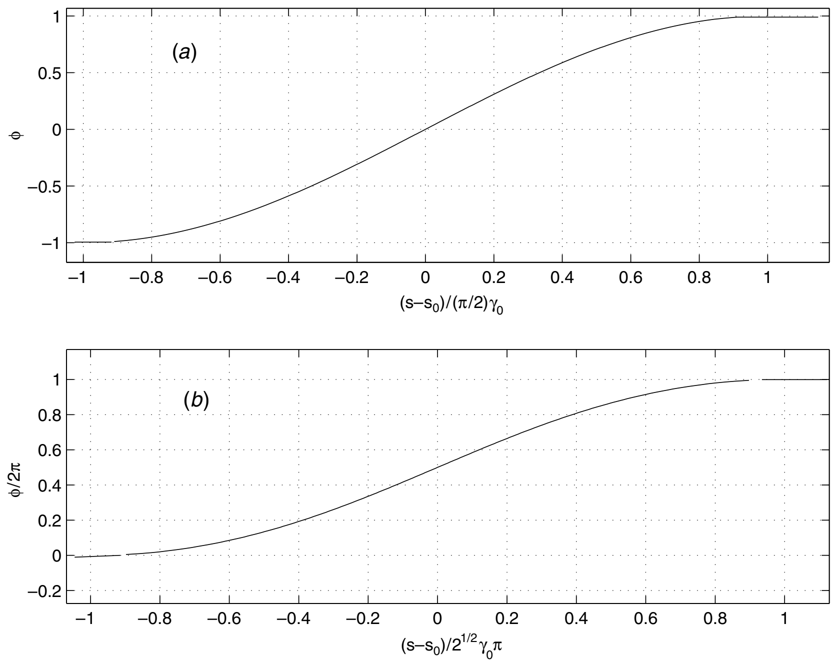

Figure 2. Kink compacton waveform: (*a*) for the ϕ-four potential and (*b*) for the sG potential.

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

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

where

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

Through a set of transformations and neglecting higher powers in (a/d_0), the transfer integral equation (3.2*a*) with the function (3.2*b*) can be approximated by a Schrödinger equation. Thus, for $C_{\mathrm{nl}} > 0$, we obtain the following Schrödinger-type equation for the eigenfunction $\Psi_n(\phi) = \exp[-\beta A a\omega_0^2 V_{\mathrm{s}}(\phi)/2]\Phi_n(\phi)$:

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

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

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

The parameters $g_1(y)$ and $g_2(y)$, defined as

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

and

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

are the renormalization parameters induced by the anharmonicity of the interparticle pair potential. $K_\ell(y)$ is the modified Bessel function of order ℓ, and y a parameter depending on the nonlinear coupling $C_{\rm nl}$, that is, $y = \beta A a C_0^4 / 8C_{\rm nl}$.

At this stage, two remarks can be made:

- Firstly, when $C_{\rm nl} = 0$ (that is $z \to \infty$), $g_1(y) = g_2(y) = 1$ and consequently $V_0 = (-1/2\rho)\ln\left(2\pi a^2/\rho d_0^2\right)$ and $m^* = (\beta A C_0 \omega_0)^2$, which are the values usually obtained in the basic NKG systems. So, the use of the TIO leads to a similar Schrödinger equation to that of the NKG systems with harmonic coupling between adjacent particles.
- Secondly, equation (3.3) can be viewed as the formal Schrödinger equation for a 'particle' of mass m^* moving in the 1D substrate potential $V_{\rm s}(\phi)$.

Hence, the classical partition function and consequently the thermodynamic properties of generalized NKG systems can be obtained easily from equations (3.1) after determining the eigenvalues $\tilde{\varepsilon}_n$ in the spirit of the basic NKG systems. For this purpose, we first evaluated $\tilde{\varepsilon}_n$.

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

$$f_l = \frac{1}{\beta a}\ln\left(\frac{\beta\hbar C_0}{a g_1(y)}\right) + A\omega_0^2\tilde{\varepsilon}_0. \tag{3.7}$$

As one can easily see, to evaluate f_l, the main problem we are faced with consists in the calculation of the lowest eigenvalue $\tilde{\varepsilon}_0$ of the Schrödinger differential operator. In the low-temperature regime $\beta \gg 1$ ($m^* \gg 1$), there are several ways to find the approximate eigenvalue $\tilde{\varepsilon}_0$, all of them known as the improved WKB methods (see [21, 22] and references therein). In the following, we use the procedure developed by Croitoru *et al* [21] based on the asymptotic methods from the theory of differential equations depending on a large parameter which for the basic NKG systems has the advantage of making a clear distinction between the various contributions to the free energy: phonons, kink, kink–kink interaction and so on. Following this procedure, the calculation of the ground state $\tilde{\varepsilon}_0$ is similar to that performed for the basic NKG systems [21, 22]. Then,

$$\tilde{\varepsilon}_0 = \tilde{\varepsilon}_{00}(1 - 2\sigma\nu), \tag{3.8}$$

with $\sigma = 1$ for the ϕ-four potential and $\sigma = 2$ for the sG potential, and where $\tilde{\varepsilon}_{00}$ is the first term in the asymptotic expansion of the lowest eigenvalue of the isolated potential well given by

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

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. The presence of these degenerate minima leads to the tunnel splitting of the lowest level $\tilde{\varepsilon}_{00}$ of the isolated well. The lower extremity can be found from the boundary conditions for the wavefunction of equation (3.3) and its derivatives. The result which takes into account the various low-lying excitation contributions is

$$\nu = \nu_{\rm k} + \nu_{\rm kk}, \tag{3.10}$$

where $\nu_{\rm k}$ may be viewed as the *single kink contribution* given by

$$\nu_{\rm k} = (6\varpi/\pi)^{1/2}\exp(-\varpi), \tag{3.11}$$

with

$$\varpi = \tfrac{2}{3}\sqrt{m^*} = \beta E_{\rm k}^0 g_2(y), \qquad E_{\rm k}^0 = \tfrac{2}{3}A C_0\omega_0, \tag{3.12}$$

for the ϕ-four potential and,

$$\nu_k = (2\varpi/\pi)^{1/2}\exp(-\varpi), \tag{3.13}$$

with

$$\varpi = 8\sqrt{m^*} = \beta E_k^0 g_2(y), \qquad E_k^0 = 8AC_0\omega_0, \tag{3.14}$$

for the sG potential, where E_k^0 is the well-known static kink energy in both cases. Note that the quantity ν_k is the tunnelling term since it follows from the escape of a particle from a potential minimum to an adjacent one. In addition, since this large displacement of particles is only assured by kink excitations, one can then interpret ν_k as the kink contribution to the expression of the eigenvalue $\tilde{\varepsilon}_0$.

The second quantity ν_{kk} which is proportional to $\exp(-2\varpi)$ may be viewed as the contribution of kink–kink interactions and is given by

$$\nu_{kk} = -\nu_k^2\ln(12\Gamma\varpi), \tag{3.15a}$$

for the ϕ-four potential and

$$\nu_{kk} = -2\nu_k^2\ln(4\Gamma\varpi), \tag{3.15b}$$

for the sG potential, where $\Gamma = 1.781\,072\ldots$ is the Euler constant. The imaginary part of ν_{kk}, that is, $(\pi/2)\nu_k^2$ for the ϕ-four potential and $\pi\nu_k^2$ for the sG potential, is omitted in the above expression and is out of the scope of this paper. Nevertheless, it can be interpreted as a quantity describing the finite lifetime of each state of the potential [10] analogous to the result of the basic NKG systems. Thus, we are now in possession of the relevant parameter $\tilde{\varepsilon}_0$ interfering in the construction of the thermodynamic properties of the system given by

$$\tilde{\varepsilon}_0 = \frac{1}{2\sqrt{m^*}} - \frac{1}{\sqrt{m^*}}\left(\frac{6\varpi}{\pi}\right)^{1/2} e^{-\varpi}[1 - \nu_k\ln(12\Gamma\varpi)], \tag{3.16}$$

for the ϕ-four potential and

$$\tilde{\varepsilon}_0 = \frac{1}{2\sqrt{m^*}} - \frac{2}{\sqrt{m^*}}\left(\frac{2\varpi}{\pi}\right)^{1/2} e^{-\varpi}[1 - 2\nu_k\ln(4\Gamma\varpi)], \tag{3.17}$$

for the sG potential. The substitution of equations (3.16) and (3.17) into equation (3.7) allows us to obtain the exact expression of the free-energy density of the system.

On the basis of the treatment of the basic NKG systems, we can then separate the free energy into two parts $f_l = f_{ph} + f_{tun}$. The first part is given by

$$f_{ph} = \frac{1}{\beta a}\ln\left(\frac{\beta\hbar C_0}{a g_1(y)}\right) + \frac{1}{2\beta d_0 g_2(y)}, \tag{3.18}$$

while the second part, which is the tunnelling contribution since it is proportional to $\exp(-\varpi)$, written in the form known from the soliton gas approach [11, 23], is given by

$$f_{tun} = -k_B T n_k(1 - Bn_k), \tag{3.19}$$

with

$$n_k = \frac{1}{d_0 g_2(y)}\left(\frac{6\beta E_k^0 g_2(y)}{\pi}\right)^{1/2}\exp\left[-\beta E_k^0 g_2(y)\right], \tag{3.20a}$$

and

$$B = d_0 g_2(y)\ln\left[12\Gamma\beta E_k^0 g_2(y)\right], \tag{3.20b}$$

for the ϕ-four potential and,

$$n_k = \frac{2}{d_0 g_2(y)}\left(\frac{2\beta E_k^0 g_2(y)}{\pi}\right)^{1/2}\exp\left[-\beta E_k^0 g_2(y)\right], \tag{3.21a}$$

and

$$B = d_0 g_2(y) \ln\left[4\Gamma\beta E_{\rm k}^0 g_2(y)\right], \tag{3.21b}$$

for the sG potential.

Note that the nonlinear interparticle coupling coefficient $C_{\rm nl}$ enters the above expressions through the effective mass m^* which depends on $C_{\rm nl}$ through the renormalization parameter $g_2(y)$. The analytical results (3.18)–(3.21*a*) are quite surprising. For a better understanding of the above expressions of the free energy, it is necessary to estimate their asymptotic analytical expressions in the limiting case of weak nonlinear coupling between adjacent particles ($C_{\rm nl} \to 0$). In this limit, equation (3.18) reduces to

$$f_{\rm ph} = \frac{1}{\beta a} \ln\left(\frac{\beta\hbar C_0}{a}\right) + \frac{1}{2\beta d_0} + \frac{3}{4}\frac{C_{\rm nl}}{\beta^2 A a^2 C_0^4}\left(1 - \frac{a}{d_0}\right), \tag{3.22}$$

where the first two terms are the well-known contribution of phonons in the free energy of the basic NKG systems. Consequently, the last term is the correction due to the anharmonicity of the interparticle potential. Indeed, if the nonlinear substrate potential is absent and the interparticle potential is harmonic, the only contribution to the free energy is that of phonons viewed as non-interacting particles. However, if the interparticle potential is anharmonic, as is the case here, the phonon–phonon interactions are produced due to the anharmonicity. In this case, the free energy is affected not only by phonons, but also by the phonon–phonon interactions. According to this result, the first part of the free energy given by equation (3.18) may be viewed as the contribution to the free energy of the generalized NKG systems of phonons and phonon–phonon interactions. The quadratic temperature dependence of the contribution of phonon–phonon interactions to the free energy, for weak nonlinear coupling ($C_{\rm nl} \to 0$), suggests that the effect of anharmonicity becomes more and more important when the temperature is increased.

We now come to the second part of the free energy. When the nonlinear interparticle coupling is weak, $g_2(y) \approx 1 + \alpha$ and then the quantity ϖ can be expanded as

$$\varpi = \beta E_{\rm k}^0(1 + \alpha), \tag{3.23}$$

where $\alpha = 3/16y = 3C_{\rm nl}/2\beta A a C_0^4$ is the renormalization constant and is linearly temperature dependent. Similarly, the quantity $n_{\rm k}$ defined by equations (3.20*a*) or (3.21*a*) can be developed as

$$n_{\rm k} = \frac{1}{d_{\rm eff}}\left(\frac{6\beta E_{\rm eff}}{\pi}\right)^{1/2} \exp(-\beta E_{\rm eff}) \approx n_{\rm k}^0\left[1 - \alpha\left(\frac{1}{2} + \beta E_{\rm k}^0\right)\right], \tag{3.24a}$$

with $n_{\rm k}^0 = (1/d_0)\left(6\beta E_{\rm k}^0/\pi\right)^{1/2} \exp\left(-\beta E_{\rm k}^0\right)$ for the ϕ-four potential and

$$n_{\rm k} = \frac{2}{d_{\rm eff}}\left(\frac{2\beta E_{\rm eff}}{\pi}\right)^{1/2} \exp(-\beta E_{\rm eff}) \approx n_{\rm k}^0\left[1 - \alpha\left(\frac{1}{2} + \beta E_{\rm k}^0\right)\right], \tag{3.24b}$$

with $n_{\rm k}^0 = (2/d_0)\left(2\beta E_{\rm k}^0/\pi\right)^{1/2} \exp\left(-\beta E_{\rm k}^0\right)$, for the sG potential. Here, the quantities $d_{\rm eff} = d_0 g_2(y) \approx d_0(1+\alpha)$ and $E_{\rm eff} = E_{\rm k}^0 g_2(y) \approx E_{\rm k}^0(1+\alpha)$ can be interpreted as the effective kink-width and kink rest-energy, respectively, and $n_{\rm k}^0$ the well-known kink density within the ideal gas approximation. So, if $C_{\rm nl} = 0$, equation (3.25*a*) reduces to the well-known kink density $n_{\rm k}^0$. The above development suggests that the quantity $n_{\rm k}$ defined by equation (3.20*a*) and (3.21*a*) for the ϕ-four potential and for the sG potential, respectively, can be interpreted as the kink density within the ideal gas approximation in the generalized NKG systems while the second part of the free energy (tunnelling term), given by equation (3.19), is the contribution of kink-phonons and kink–kink interactions. Accordingly, the logarithmic temperature dependence quantity B defined by equations (3.20b) and (3.21b), which designates the second virial coefficient in the free energy, can also be attributed to the spatial shift in the trajectory of kink solitons caused by an elastic collision [11, 23]. It can also be written in the compact form as

$$B = d_{\text{eff}} \ln(12\Gamma\beta E_{\text{eff}}), \tag{3.25a}$$

for the ϕ-four potential and

$$B = d_{\text{eff}} \ln(4\Gamma\beta E_{\text{eff}}), \tag{3.25b}$$

for the sG potential. It appears that the nonlinear interparticle coupling contributes to increasing the second virial coefficient. Consequently, one can conclude that the anharmonicity of the interparticle potential contributes to the increase of the kink–kink interactions in the system.

Actually, what the above results suggest is that, the temperature enters n_{k} through the ratio βE_{k}^0 and also through the parameter y. Thus, the universal temperature dependence of the low-temperature density of kinks $n_{\text{k}} \propto (\beta E_{\text{k}})^{1/2} \exp(-\beta E_{\text{k}})$ with E_{k} being the static kink energy, where only numerical prefactors are model dependent and where the temperature enters only through the ratio βE_{k}, is longer more valid when the anharmonicity of the interparticle pair potential is taken into account, since E_{k} has been replaced by the temperature-dependent static kink effective energy E_{eff}.

As we have calculated the free-energy density f_l, all other thermodynamic quantities such as the internal energy, the entropy and the specific heat capacity can be readily obtained. For example, in the limit of weak anharmonicity of the interparticle pair potential and where B is negligible, the specific heat per particle is given by

$$\begin{aligned} c_N/k_{\text{B}} = 1 - \alpha(1 - a/d_0) + n_{\text{k}}^0 a\left[\left(\beta E_{\text{k}}^0 - 1/2\right)^2 - 1/2\right] \\ - n_{\text{k}}^0 a\alpha\left(\beta E_{\text{k}}^0 + 1/2\right)\left[\left(\beta E_{\text{k}}^0 - 1/2\right)^2 + 1/2\right]. \end{aligned} \tag{3.26}$$

The terms proportional to α are the correction factors due to the anharmonicity of the interparticle pair potential. It appears that the anharmonicity of the interparticle potential contributes in lowering the specific heat.

We now turn our attention to one of the important cases, that is, the purely anharmonic system ($C_0 = 0$). In this limit, as mentioned in section 2, the system exhibits the static kink compacton. So, one may expect that the thermodynamic properties of the system can be influenced by the existence of this static kink compacton. In fact, in the limit $C_0 = 0$, the TIO (3.2a) can also be approximated, in the limit of slowly varying fields ($d_{\text{kc}} \gg a$), by the Schrödinger equation (3.3) with characteristic parameters m^* and V_0 given by

$$\begin{aligned} m^* &= \beta A a\omega_0^2 \frac{\Gamma(1/4)}{\Gamma(3/4)} \left(\frac{\beta A C_{\text{nl}}}{4a^3}\right)^{1/2}, \\ V_0 &= -\frac{1}{2\beta A a\omega_0^2} \ln\left[\frac{\sqrt{2}}{4}\Gamma(1/4)^2 \left(\frac{a^3}{\beta A C_{\text{nl}}}\right)^{1/2}\right]. \end{aligned} \tag{3.27}$$

By making use of the procedure of the preceding paragraph for solving $\tilde{\varepsilon}_0$, we then arrive at the following mathematical expressions of $\tilde{\varepsilon}_0$:

$$\tilde{\varepsilon}_0 = \frac{1}{2\sqrt{m^*}} - \frac{1}{\sqrt{m^*}} \left(\frac{6\varpi}{\pi}\right)^{1/2} \mathrm{e}^{-\varpi}[1 - \nu_{\text{k}} \ln(12\Gamma\varpi)], \tag{3.28a}$$

for the ϕ-four potential and

$$\tilde{\varepsilon}_0 = \frac{1}{2\sqrt{m^*}} - \frac{2}{\sqrt{m^*}} \left(\frac{2\varpi}{\pi}\right)^{1/2} \mathrm{e}^{-\varpi}[1 - 2\nu_{\text{k}} \ln(4\Gamma\varpi)], \tag{3.28b}$$

for the sG potential. These expressions of $\tilde{\varepsilon}_0$ are similar to those obtained for the kink soliton bearing systems given by equations (3.16) and (3.17), and for which the quantities m^* and ϖ are expressed in a different manner. Thus, we have

$$\varpi = \chi[\beta E_{\rm kc}]^{3/4}, \tag{3.29}$$

where χ is a temperature-independent coefficient given by

$$\chi = \left\{ \frac{2^{13}}{3^5\pi^4} \left[\frac{\Gamma(1/4)}{\Gamma(3/4)} \right]^2 \left(\frac{d_{\rm kc}}{a} \right) \right\}^{1/4}, \tag{3.30a}$$

for the ϕ-four potential, and

$$\chi = \left\{ \frac{2^{3/4}3^5}{\pi^{5/2}} \frac{\Gamma(3/4)}{\Gamma(1/4)} \left(\frac{d_{\rm kc}}{a} \right) \right\}^{1/4}, \tag{3.30b}$$

for the sG potential, and where $E_{\rm kc}$ is the static kink compacton energy defined by equation (2.7) for the ϕ-four potential and by equation (2.8b) for the sG one.

By substituting equation (3.28a) into equation (3.1) and evaluating $f_l = (1/\beta L)\ln Z$, we obtain the exact analytical free-energy density of the purely anharmonic system coming from the Hamiltonian (2.1). This expression can be separated into two parts: $f_l = f_{\rm ph} + f_{\rm tun}$, where $f_{\rm ph}$ can be viewed as the contribution of anharmonic phonons to the free energy:

$$f_{\rm ph} = \frac{1}{4\beta a} \ln\left[\frac{2\beta^3 h^4 C_{\rm nl}}{\Gamma(1/4)^4\pi^2 A a^5} \right] + \left[\frac{\Gamma(3/4)}{2\Gamma(1/4)} \right]^{1/2} \left[\frac{A a \omega_0^2}{\beta^3 C_{\rm nl}} \right]^{1/4}, \tag{3.31}$$

while the tunnelling part, $f_{\rm tun}$, which is a function of kink compacton parameters, can be written as

$$f_{\rm tun} = -k_{\rm B} T n_{\rm kc}(1 - B_{\rm kc} n_{\rm kc}), \tag{3.32}$$

in analogy with the tunnelling part of basic NKG systems, with

$$n_{\rm kc} = \left(\frac{2^{11}}{3\pi} \right)^{1/2} \frac{(\beta E_{\rm kc})^{5/8}}{\chi^{1/2} d_{\rm kc}} \exp[-\chi(\beta E_{\rm kc})^{3/4}], \tag{3.33}$$

$$B_{\rm kc} = \frac{3}{32}\chi(\beta E_{\rm kc})^{-1/4} d_{\rm kc} \ln[12\Gamma\chi(\beta E_{\rm kc})^{3/4}], \tag{3.34}$$

for the ϕ-four potential and

$$n_{\rm kc} = 9 \times 2^{3/4} \left[\frac{\Gamma(3/4)}{\Gamma(1/4)} \right] \frac{(\beta E_{\rm kc})^{5/8}}{\chi^{1/2} d_{\rm kc}} \exp[-\chi(\beta E_{\rm kc})^{3/4}], \tag{3.35}$$

$$B_{\rm kc} = \frac{2^{3/4}}{3^2\sqrt{\pi}} \frac{\Gamma(1/4)}{\Gamma(3/4)} \chi\left(\beta E_{\rm kc}^{(c)}\right)^{-1/4} d_{\rm kc} \ln\left[4\Gamma\chi\left(\beta E_{\rm kc}^{(c)}\right)^{3/4}\right], \tag{3.36}$$

for the sG potential.

Equations (3.32)–(3.36) give the exact result of the free-energy density. However, it is not possible to give here with certainty the correct interpretation of quantities $n_{\rm kc}$ and $B_{\rm kc}$, since we are not in possession of the phenomenological results of kink compacton gas like those resulting from the CKBT theory of kink soliton gas. Nevertheless, based on the results of the soliton gas approach, we may interpret $n_{\rm kc}$ as the kink compacton density within the ideal gas of kink compactons. Although the first term of the tunnelling contribution of the free energy density of the system verifies a temperature dependence relation similar to that of kink solitons where numerical prefactors are model dependent and where the temperature enters the kink density only through the ratio $\beta E_{\rm kc}$, the power of the ratio $\beta E_{\rm kc}$ appearing in the

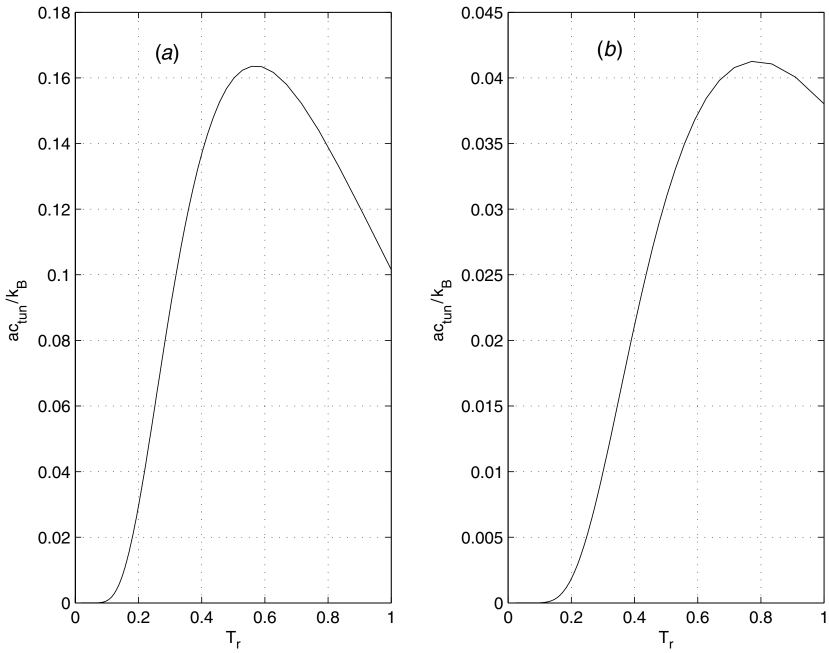

Figure 3. Specific heat of kink compactons (c_{tun}) as a function of the reduced temperature $T_r = k_B T/E_{\text{kc}}$: (*a*) for the ϕ-four potential and (*b*) for the sG potential, with $d_{\text{kc}}/a = 10$. c_{tun} is the last term of equation (3.39) which is proportional to n_{kc} and E_{kc} is the static kink compacton energy.

Arrhenius factor of n_{kc} or of the exact result of the free energy density is 3/4 instead of 1. In addition, in this Arrhenius factor a numerical temperature independent coefficient χ appears which is inversely proportional to the dimensionless discreteness parameter (a/d_{kc}) of purely anharmonic systems.

As we have calculated the free energy density, all other thermodynamic quantities can be readily obtained. The internal energy density $u = U/L = \partial\beta f/\partial\beta$, in the limit of weak B_{kc}, is given by

$$u = \frac{1}{\beta a}\left\{\frac{3}{4} + \frac{1}{8}\left(\frac{24}{\eta}\right)^{1/4}\left[\frac{\Gamma(3/4)}{\Gamma(1/4)}\right]^{1/2}\frac{a}{\gamma}\left(\beta A a\omega_0^2\right)^{1/2}\right\} - \frac{n_{\text{kc}}}{\beta}\left[\frac{5}{8} - \frac{3}{4}\chi\left(\beta E_{\text{kc}}\right)^{3/4}\right], \tag{3.37}$$

while the entropy is easily found to have the form:

$$s/k_B = \frac{1}{4a}\left\{3 - \ln\left[\frac{4\beta^3 h^4 C_{\text{nl}}}{\pi^2\Gamma(1/4)^4 A a^5}\right]\right\} - \frac{3}{8}\left(\frac{24}{\eta}\right)^{1/4}\left[\frac{\Gamma(3/4)}{\Gamma(1/4)}\right]^{1/2}\frac{1}{\gamma}\left(\beta A a\omega_0^2\right)^{1/4} + \frac{3}{4}n_{\text{ck}}\left[\frac{1}{2} + \chi\left(\beta E_{\text{kc}}\right)^{3/4}\right] \tag{3.38}$$

and the specific heat per unit length has the form

$$c/k_B = \frac{3}{4a}\left\{\frac{1}{4} + \frac{1}{8}\left(\frac{24}{\eta}\right)^{1/4}\left[\frac{\Gamma(3/4)}{\Gamma(1/4)}\right]^{1/2}\frac{a}{\gamma}\left(\beta A a\omega_0^2\right)^{1/4}\right\} + n_{\text{kc}}\left\{\left[\frac{3}{4}\chi\left(\beta E_{\text{kc}}\right)^{3/4} - \frac{1}{2}\right]^2 - \frac{31}{64}\right\}. \tag{3.39}$$

The terms proportional to n_{kc} are the tunnelling contributions and result from the presence of kink compactons in the system. All of these thermodynamic functions are of course functions of the kink compacton parameters, namely, the width and static energy. Figure 3 shows, for example, the variation of the tunnelling contribution of the specific heat of the system as a function of the temperature. As the temperature is increased, it varies and reaches a maximum. This behaviour of the tunnelling contribution of the specific heat has already been observed in the kink soliton-bearing systems.

4. Conclusion

As is well known, the TIO method gives rise to the exact calculation of the thermodynamic properties at low temperature of Hamiltonian systems including kink-bearing systems. Since NKG systems with anharmonic interparticle potential exhibit a rich variety of static and travelling solitonic structures among which are the kink solitons and kink compactons, in this paper, we have investigated the low-temperature statistical mechanics of these systems by means of the TIO method. The exact explicit expression of the free energy has been obtained. We have shown that in the limit of weak nonlinear interparticle coupling, the anharmonicity of the interparticle potential contributes to lowering the specific heat, and the associated dimensionless renormalization constant α linearly depends on the temperature. Thus, the effect of anharmonicity becomes more and more important when the temperature is increased. In addition, for arbitrary nonlinear interparticle coupling, although the presence of kink solitons still remains signalled by an exponential term $\exp(-\beta E_k)$, nevertheless, the quantity E_k appears to be the effective static energy of the kink soliton which is a complicated function of the temperature. Interestingly, for purely anharmonic systems, the presence of kink compactons is signalled by a term proportional to $\exp[-\chi(\beta E_{kc})^{3/4}]$ in the free energy density where E_{kc} is the energy of the static kink compacton and χ a coefficient inversely proportional to the dimensionless discreteness parameter of the system.

Although a complete proof of a similar CKBT phenomenology does not exist at present, the exact results of thermodynamic quantities obtained here strongly support the idea that their phenomenology should be valid at low temperatures. We hope that these exact results for 1D NKG systems with anharmonic interparticle interactions and those of the kink compacton-bearing systems will stimulate further studies with the goal of making detailed comparisons to test the validity of a further phenomenological generalization of the CKBT theory. Let us mention that our results are valid only when the nonlinear interparticle coupling has positive values ($C_{nl} > 0$). However, as the negative values of C_{nl} provide additional attractive or repulsive interactions between sites which are responsible for the appearance of solitonic structures such as defects, bubbles, peakons and cups [15], it would then be necessary to extend this work to this particular case, which is now under consideration.

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