Dynamics and thermodynamics of the sine-Gordon system with long-range interaction potential

1994 J. Phys.: Condens. Matter 6 4277

(http://iopscience.iop.org/0953-8984/6/23/007)

J. Phys.: Condens. Matter 6 (1994) 4277–4288. Printed in the UK

Dynamics and thermodynamics of the sine–Gordon system with long-range interaction potential

J R Kenné, P Woafo and T C Kofané

Laboratoire de Mécanique, Faculté des Sciences, Université de Yaoundé I, BP 812 Yaoundé, Cameroun

Received 13 August 1993

Abstract. The dynamics and thermodynamic properties of the sine–Gordon system with the Kac–Baker long-range interaction are considered. The dispersion relations are derived and a closed-form kink solution is obtained. It appears that the kink width and energy increase as the range of interaction increases. Using a suitable conversion of the functional integral, the transfer matrix techniques are used to evaluate the classical thermodynamic properties of the model in the low-temperature regime. They are seen to depend strongly on the range of interaction.

1. Introduction

The dynamics and thermodynamics of non-linear lattices with long-range interaction potential have received a great deal of attention in the past decade [1–12]. Such attention is due to the fact that, in certain real materials, the interparticle forces extend further than the nearest-neighbour interactions, for instance, in metal or ferroelectric chains [6] and in adsorption systems where adatomic charges create Coulomb repulsion forces, dipole–dipole interaction and direct or indirect interaction [7].

The long-range (or non-local) interaction potential is generally complicated, but some interesting forms are known and have been studied: power-law interaction [3, 7], Lennard-Jones long-range coupling [2] and exponential interaction such as Kac–Baker potential [13]. This last potential is described in section 2 of the present paper.

The interplay between the long-range interaction and non-linearity has revealed interesting new phenomena from both the mathematical and physical points of view: the generation of new types of solitons and the coexistence of supersonic and subsonic solitons in a given lattice [2, 4, 14, 15]; the blow-up or the splitting of solitons due to competition (frustration) between the first- and second-nearest interactions [14, 15]; the explanation of the observed finite exponent that appears on the density of solitons at zero temperature [3]; the increase of soliton width with the range of interaction [1, 4]; the decreasing behaviour of the Peierls–Nabarro barrier associated with kinks in the discrete lattice [8, 16]; and finally the decrease of kink free energy and density when the range of interaction increases [9].

Owing to the mathematical complexity, the connection between the long-range interaction potential and the widely used sine–Gordon (SG) substrate potential has received limited investigation. To our knowledge, the first study dealing with such a connection was carried out by Pokrovsky and Virosztek [3], who used an integral operator that contains both the short-range (local) and the long-range (non-local) interactions to analyse the problem, as mentioned here before, of the finite exponent observed in the soliton density at zero temperature. Braun *et al* [7] have considered the Frenkel–Kontorova systems with

0953-8984/94/234277+12$19.50

power-law interaction and Kac–Baker potential. Taking the Kac–Baker interactions as perturbations, they found a renormalization of kink parameters. In a letter published recently [17], we have derived an implicit form for topological solitons in a SG system with the Kac–Baker potential. The thermodynamic properties and the existence of other types of excitations were still to be analysed. This constitutes the aim of the present paper.

In section 2, we review the model and present the resulting linear and non-linear excitations. The dispersion relations for phonons are derived and additional developments for the kink solutions are given. In section 3, the transfer integral techniques are used to derive the partition function by suitably converting the functional integral into an equivalent nearest-neighbours problem. From this, we find the low-temperature properties of the system. These properties (free energy, internal energy, specific heat, entropy and density of kinks) are discussed with respect to the range of interaction. The concluding remarks and suggestions for future investigations are reported in section 4.

2. Model and excitations

We consider a system of particles of mass m placed on an infinite one-dimensional lattice. Each particle is lying on an on-site potential $V(\phi_i)$. The Hamiltonian of such a system is then given by

$$H = \tfrac{1}{2}m\sum_i \dot{\phi}_i^2 + \sum_i V(\phi_i) + \tfrac{1}{2}\sum_{i\neq j} V_{ij}(\phi_i - \phi_j)^2 \tag{1}$$

where i, j are the lattice points; ϕ_i and $\dot{\phi}_i$ are respectively the linear displacement and the velocity of the ith particle; m is the mass of the particle; and V_{ij} is the Kac–Baker potential [13] in which the interaction between particles falls off exponentially as the separation increases. The latter is defined as

$$V_{ij} = [c(1-r)/2r]r^{|i-j|} \tag{2}$$

where the coefficient c is the elastic constant of the lattice (or the exchange constant in magnets), and the absolute difference $|i-j|$ measures the distance between sites i and j. Experimentally, one can relate the parameter r to the number of neighbouring interactions [11]. Particular interest devoted to the potential (2) is reported in [9] and [17]. The substrate potential $V(\phi_i)$ is of the sine–Gordon (SG) type, that is

$$V(\phi_i) = \alpha[1 - \cos(2\pi\phi_i/b)] \tag{3}$$

where α is the amplitude of the SG substrate potential and b is the lattice constant.

Putting $u_i = 2\pi\phi_i/b$, the equation of motion that follows from (1), (2) and (3) is

$$M\ddot{u}_i + \alpha \sin u_i + 2Cu_i = L_i \tag{4}$$

where

$$M = b^2m/4\pi^2 \qquad C = b^2c/4\pi^2$$

and the auxiliary quantity L_i defined as

$$L_i = \frac{C(1-r)}{r}\sum_{i\neq j} r^{|i-j|}u_j \tag{5}$$

satisfies the following recursive relation

$$(r + r^{-1})L_i = L_{i+1} + L_{i-1} + [C(i - r)/r](u_{i+1} + u_{i-1} - 2ru_i). \tag{6}$$

In the continuum limit, the discrete set of equations (4) reduces to the partial differential equation

$$Mrb^2u_{2x2t} + \alpha rb^2(\sin u)_{2x} + C(1 + r)b^2u_{2x} - (1 - r)^2(Mu_{2t} + \alpha \sin u) = 0. \tag{7}$$

The $2x$ (or $2t$) stands for the partial spatial (or time) derivative. For $r = 0$, equation (7) reduces to the well known continuum SG equation [19]. An equation similar to (7) was also derived by Roseneau [5] for a weakly non-linear one-dimensional lattice with N neighbouring interactions by using a method that correctly preserves the essential features of the discrete system. But no special link was assumed between the coupling coefficients of different neighbouring interactions. Consequently, the coefficient of the u_{2x2t} term, as well as that of the non-linear interaction potential term, were given as sums over the N interacting particles. But, in our equation (7), the coefficient of u_{2x2t} depends on the parameter r, which measures the range of interaction. This is due to the exponential form (link) of the elastic coupling coefficients between all the particles of the lattice.

The discrete set of equations (4) and its continuum form (7) have two trivial solutions, which correspond to the unstable state $u_i = (2n + 1)\pi$ (or $u = (2n + 1)\pi$) and the stable state $u_i = 2n\pi$ (or $u = 2n\pi$), where n is an integer. These equations (4) and (7) also admit small-amplitude solutions (the so-called phonons) and large-amplitude solutions (the kink and antikink) [17].

2.1. Discrete and continuum phonons

2.1.1. Oscillations about $u_i = 2n\pi$. This case corresponds to the state where all the particles are lowered to the bottom of the substrate potential wells and because of small disturbances (e.g. small thermal fluctuations) undergo oscillatory motion with displacements

$$u_i = a \sin(kb_i - \omega_k t) \tag{8a}$$

where a is the amplitude, k the wavenumber and ω_k the oscillatory frequency. To find the dispersion relation to this phonon state, we use the recursive relation (4) in equation (6) to obtain in the linear order

$$(1+r^2)M\ddot{u}_i - rM(\ddot{u}_{i+1} + \ddot{u}_{i-1}) = [C(1+r)+\alpha r](u_{i+1} + u_{i-1}) - [2C(1+r)+\alpha(1+r^2)]u_i. \tag{8b}$$

Inserting (8*a*) into (8*b*), the dispersion relation becomes

$$\omega_k^2 = \frac{[2C(1 + r) + 2\alpha r]\cos(kb) - 2C(1 + r) - \alpha(1 + r^2)}{M[2r\cos(kb) - (1 + r^2)]}. \tag{9a}$$

When the wavenumber k is small, equation (9*a*) takes the form

$$\omega_k^2 = \frac{(kb)^2[C(1 + r) + r\alpha] + \alpha(1 - r)^2}{M[(1 - r)^2 + r(kb)^2]} \tag{9b}$$

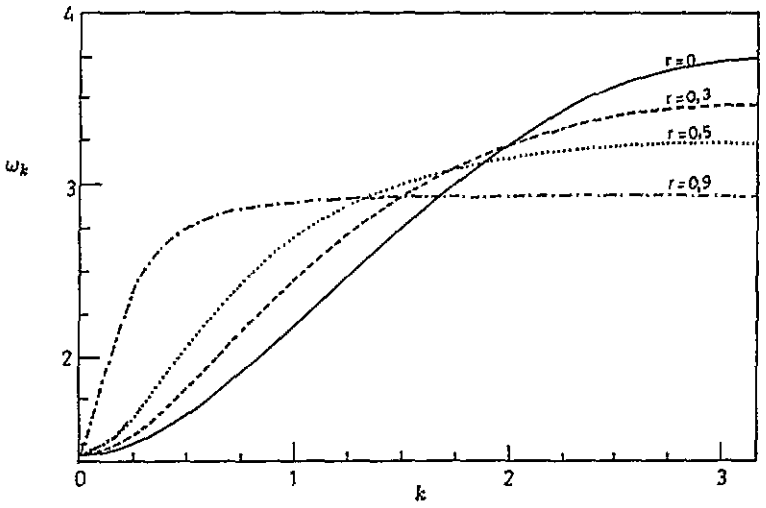

Figure 1. Dispersion relation for various values of the interaction parameter r ($C = 3$, $\alpha = 2$, $M = 1$).

which is the continuum dispersion relation of the model, also obtainable by linearization of equation (7). This relation (*9b*) shows that ω_k^2 is always positive. When $r \to 0$, the relations (*9a*) and (*9b*) reduce to the discrete and continuum relations of the SG chain with the first-neighbour interaction [19].

In figure 1, we plot in the first Brillouin zone the dispersion relation for various values of the interaction parameter r. This figure leads to the following comments: In the domain of wavenumber k near $k = 0$, it is seen that, for a given wavenumber, the wave dispersion increases when r increases. This is in agreement with the fact that, in the continuum limit, the long range increases the dispersion of waves [2]. However, in the second domain near $k = \pi/b$ (the discrete limit), an inverse phenomenon is observed. This leads to the decrease of dispersion when the range of interaction decreases. The shape of this figure is qualitatively similar to that of the experimental dispersion relation in plumb where the long-range interaction exists [11].

2.1.2. Oscillation about $u_i = (2n + 1)\pi$. This corresponds to the situation in which all the particles sit in the tops of the wells. Then we can write $u_i = (2n + 1)\pi + V_i$, where V_i is a linear wave. Substitution in equation (8) leads to

$$(1+r^2)M\ddot{V}_i - rM(\ddot{V}_{i+1} + \ddot{V}_{i-1}) = [C(1+r) - \alpha r](V_{i+1} + V_{i-1}) - [2C(1+r) - \alpha(1+r^2)]V_i \tag{10}$$

and the discrete dispersion relation in this state is then given by

$$\omega_k^2 = \frac{[2C(1+r) - 2\alpha r]\cos(kb) - 2C(1+r) + \alpha(1+r^2)}{M[2r\cos(kb) - (1+r^2)]}. \tag{11a}$$

When $k \to 0$, this equation reduces to

$$\omega_k^2 = \frac{(kb)^2[C(1+r) - r\alpha] - \alpha(1-r)^2}{M[(1-r)^2 + r(kb)^2]}. \tag{11b}$$

For the stability of linear oscillations about the top of SG potential wells, ω_k^2 should be positive. This leads to the following inequality

$$k^2 > \frac{\alpha(1-r)^2}{b^2[C(1+r)-r\alpha]} \tag{11c}$$

for the wavenumber k (assuming that the right-hand side of (11*c*) is positive, this requires $C > \alpha$).

2.2. *Large-amplitude solutions*

The large-amplitude excitations in the displacive limit, corresponding to solutions of equation (7), have been derived recently [17] using the procedure of [1]. They correspond to the state where the particles have enough energy to pass gradually over the barrier of the substrate potential. These excitations called kinks or antikinks have the closed-form expression (see [17])

$$\pm\frac{x-vt}{\xi} = \frac{(1+\sigma)^{1/2}}{2} \times \ln\left(\frac{2\sin^2(u/2)}{2+2(1+2\sigma)\cos^2(u/2)+4\{(1+\sigma)[1+\sigma\cos^2(u/2)]\cos^2(u/2)\}^{1/2}}\right) - \sigma^{1/2}\ln[[4\{\sigma[1-\sigma\cos^2(u/2)]\cos^2(u/2)\}^{1/2} - 2[1+2\sigma\cos^2(u/2)]]] \tag{12a}$$

where

$$\xi^2 = [C(1+r)b^2 - mv^2(1-r)^2]/\alpha(1-r)^2 \tag{12b}$$

and σ is a positive parameter defined as

$$\sigma = r\alpha b^2/[C(1+r)b^2 - mv^2(1-r)^2]. \tag{12c}$$

In equation (12*a*) the + sign corresponds to a kink while the − sign corresponds to an antikink.

As $r \to 0$, $\sigma \to 0$, and the implicit solution (12) reduces to the standard SG kink

$$u = 4\tan^{-1}\left[\exp\left(\pm\frac{x-vt}{d(1-v^2/c_0^2)^{1/2}}\right)\right] \tag{13}$$

with $c_0^2 = Cb^2/M$ and $d^2 = Cb^2/\alpha$.

The parameter ξ gives a measure of the soliton width. It increases with r and the soliton slowly disappears. Since the kink width ξ should be greater than the lattice spacing b (in view of the continuum approximation to be satisfied), the soliton equation (12*b*) requires that $C > \alpha$ and the parameter σ therefore varies from zero to one.

In the limit $r \to 1$ the soliton extension goes to infinity (diverges as $(1-r)^{-1}$) and $u \to \pi$ for all x. This corresponds to the case in which all the particles sit at the top of the well of the SG substrate potential and have maximum energy. At this point of the substrate potential, they can oscillate with the dispersion relation (11*a*).

The stability of kinks has appeared to be an analytically difficult task owing to the complexity of the analysis. However, the Goldstone mode was obtained and other particular cases were studied [17].

2.3. Energy of the kink

Using the auxiliary quantity L_i, equation (4) and going to the continuum limit, the total energy E_s, of the soliton has the form (see [17])

$$E_s = \alpha\sigma\xi(1+\sigma)^{1/2} + \left(\frac{4Mv^2}{\xi\sigma^2} + \frac{2\alpha\xi}{\sigma^{1/2}} - 4\alpha\xi\sigma^{1/2}\right)\ln[(1+\sigma)^{1/2} + \sigma^{1/2}]$$
$$+ \frac{4Mv^2}{\xi}\left(\frac{(1+\sigma)}{\sigma(1-\sigma)}\right)\tan^{-1}\left(\frac{\sigma}{1-\sigma}\right)^{1/2}. \tag{14}$$

Analysis of equation (14) shows that E_s goes to infinity as $r \to 1$. This state, as mentioned earlier, is energetically less favourable for the existence of the soliton since all the particles sit at the top of the well (an unstable position). The variation of the soliton energy shows that E_s increases with r (see [17]).

When $r \to 0$, σ remains a small parameter, and we can expand equation (14) in powers of σ. To second order, we have

$$E_s = \alpha\xi(8 - \tfrac{4}{3}\sigma + \tfrac{1}{2}\sigma^{3/2}) + (Mv^2/\xi)(8 + 4\sigma + \sigma^{3/2} + \tfrac{5}{3}\sigma^2). \tag{15}$$

In the limit $r = 0$, E reduces to

$$E_s = 8b(\alpha C)^{1/2}/(1 - v^2/c_0^2)^{1/2} \tag{16}$$

which corresponds to the well known relativistic kink energy of the SG model with nearest-neighbour interactions [19].

3. Statistical mechanics

In this section we concentrate on the thermodynamic quantities of the long-range interaction model. The partition function and the associated properties such as the free energy, the internal energy, the specific heat and the entropy are derived and their dependence on the long-range parameter r is discussed. To this aim, we use the transfer matrix techniques [20] to reduce the functional integration to a one-particle quantum-mechanical problem. Owing to the difficulties of dealing with interactions of various types of excitations, in the long-range interaction model (kink–kink, kink–phonon or kink–breather interactions), we restrict our analysis to the case of a gas of independent kinks (antikinks) and phonon excitations.

The partition function can be written as a functional integral of the form

$$Z = \int_{-\infty}^{+\infty} \prod_{i=1}^{N} \mathrm{d}u_i \prod_{i=1}^{N} \mathrm{d}P_i \exp[-\beta H(P_i, u_i)] \tag{17}$$

where $P_i = m\dot{u}_i$ is the momentum of the ith particle, $\beta = 1/K_B T$ is the Boltzmann factor and N is the number of particles.

Since our analysis is for a classical field, equation (17) can be separated into a product of the kinetic and configurational partition function Z_p and Z_u. The kinetic part Z_p associated with the N momenta P_i of the particles, can easily be evaluated and yields

$$Z_p = (2\pi M/\beta)^{N/2}. \tag{18}$$

The configurational partition function Z_u is defined as

$$Z_u = \int_{-\infty}^{+\infty} \cdots \int \left(\prod_i^N du_i \right) \exp[-\beta W(u_i)] \tag{19}$$

where $W(u_i)$, standing for the potential energy of a given particle in a system with long-range interaction, has the form

$$W(u_i) = \alpha(1 - \cos u_i) + \frac{1}{2} \frac{C(1-r)}{2r} \sum_{i \neq j} r^{|i-j|}(u_i - u_j)^2. \tag{20}$$

We can rewrite Z_u according to (20) as

$$Z_u = \int_{-\infty}^{+\infty} \cdots \int \left(\prod_i^N du_i \right) \exp[-\beta W'(u_i)] \exp\left(\frac{K(1-r)}{r} \sum_{j>i} u_i u_j r^{|i-j|} \right) \tag{21}$$

with $W'(u_i) = \alpha(1 - \cos u_i) + Cu_i^2$ and $K = \beta C$.

Using the auxiliary field variable y_i as defined in [1], the partition function can be transformed to the equivalent nearest-neighbours problem. The kernel function is given by

$$G(y, y') = \exp[-\beta W'(y - ry') + K(1-r)y'(y - ry')]. \tag{22}$$

Since the kernel is not symmetric in y and y', we express it in terms of left and right eigenvectors. Assuming the normalization condition, the eigenvalues λ_m are defined as

$$\lambda_m \phi_m = \int_{-\infty}^{+\infty} dy' \, G(y, y') \phi_m(y') \tag{23}$$

where ϕ_m are eigenvectors.

In the thermodynamic limit, we obtain

$$Z_u = \lambda_0 \tag{24}$$

where λ_0 is the largest eigenvalue of equation (23).

When r is equal to zero, equation (23) reduces to

$$\lambda_m \phi_m(y) = \int_{-\infty}^{+\infty} dy' \, \exp[-\alpha'(1 - \cos y) - Ky'^2 + Kyy'] \phi_m(y') \tag{25}$$

where $\alpha' = \beta\alpha$. The kernel is not symmetric, and we define the transformation

$$\phi_m(y) = \exp[\alpha'(1 - \cos y) + \tfrac{1}{2} K y^2] h_m(y). \tag{26}$$

After substitution in equation (25), it appears that $h_m(y)$ satisfies

$$\lambda_m h_m(y) = \exp[-\alpha'(1 - \cos y)] \int_{-\infty}^{+\infty} dy' \, \exp[-\tfrac{1}{2} K(y - y')^2] h_m(y'). \tag{27}$$

This is the integral equation for the short-range problem. It can be easily converted into an effective Schrödinger equation valid for small θ ($\theta = \alpha/C$).

As the symmetry of the kernel is not assumed for finite r, the simplification is impossible. To evaluate the low-temperature properties, we define the transformation

$$\phi_m(y) = \exp\{\alpha'(1-r)^2 \cos y - K[r^2 - \tfrac{1}{2}(1+r)]y^2\}. \tag{28}$$

After substitution in equation (23), it appears that $h_m(y)$ satisfies

$$\lambda_m h_m(y) = \int_{-\infty}^{+\infty} dy' \exp[-\alpha'[1-\cos(y'-ry)] + \alpha'(1-r)^2(\cos y' - \cos y)] \times \exp[-\tfrac{1}{2}K(1+r)(y'-y)^2] h_m(y'). \tag{29}$$

In this relation, only the term $\cos(y'-ry)$ is not symmetric. This is a consequence of the transformation (28) which has the property of making the kernel as symmetric as possible (for instance, the kernel is symmetric for the limiting cases $r = 0$ and $r = 1$). Assuming, therefore, the asymmetry of the kernel (at least for small values of r), we derive the Schrödinger equation. Following the method of Sarker and Krumhansl [1], we obtain

$$\left(-\frac{1}{2M^*}\frac{d^2}{dx^2} + \alpha(1-\cos x)\right) h_m(x) = \epsilon_m h_m(x) \tag{30}$$

where $x = (1-r)y$, $M^* = \beta^2 \xi_0^2 \alpha$ and ξ_0 is the soliton width with the zero velocity $v = 0$.

The largest eigenvalue λ_0 of the integral equation corresponds to the ground-state energy of equation (30). It can be related to the eigenvalue of the Schrödinger equation by the formula

$$\lambda_m = (2\pi\eta)^{1/2} \exp(-\beta\epsilon_m) \tag{31}$$

where

$$\eta = [K(1-r)]^{-1}.$$

Since the potential in equation (30) is periodic with period 2π, the above equation is the familiar Hill (or Mathieu) equation of the band theory of solids. A similar equation was also analysed by Gupta and Sutherland for a general periodic potential [21]. In the low-temperature regime ($\beta E_s^{(0)} \gg 1$), the eigenspectrum will be 'tunnel-split' to remove degeneracy from the eigenstates of individual wells. If $E_0(T)$ is the lowest level in a single isolated well, then

$$\epsilon_0 = E_0(T) - t_0 \tag{32}$$

where t_0 is the tunnelling component, which is given by a standard Wentzel–Kramer–Brillouin (WKB) formula [19]

$$t_0 = [E_0(T)/\pi] \exp[-I(T)]$$

with

$$I(T) = (2m^*)^{1/2} \int_{X_1+\delta X_1(T)}^{X_2-\delta X_2(T)} dX\, |E_0 - \alpha(1-\cos X)|^{1/2} \tag{33}$$

where X_1 and X_2 define the 'turning points'. At sufficiently low temperature, $E_0(T)$ is approximated by the lowest harmonic oscillator level.

Asymptotic expansions are available for the position and width of the bands of equation (30). For $4M^* \gg 1$, the bottom of the lowest band is given by [22, 23]

$$\epsilon_0 = \frac{1}{2\beta\xi} - \frac{1}{32\alpha^2\beta^2\xi^2} - \frac{1}{512\alpha^3\beta^3\xi^3} - \frac{16\alpha\sqrt{2}}{\sqrt{\pi}}(\beta E_s^{(0)})^{-1/2}\exp(-\beta E_s^{(0)}) \tag{34}$$

where $E_s^{(0)} = 8\alpha\xi$ is the soliton rest energy. The first term of the power series represents the phonon contribution, while the higher-order terms are anharmonic contributions.

In the low-temperature regime, the free energy f per particle is given by

$$\beta f = -\tfrac{1}{2}\ln(2\pi/\beta) - \ln\lambda_0. \tag{35}$$

Using equations (31), (34) and (35), we obtain

$$f = \frac{1}{\beta}\ln\left(\frac{\beta\xi(1-r)\omega_0}{2\pi b}\right) + \frac{1}{2\beta\xi} - \frac{2}{(\beta E_s^{(0)})^2} - \frac{1}{(\beta E_s^{(0)})^3} - \frac{4}{\beta\xi\sqrt{(2\pi)}}(\beta E_s^{(0)})^{-1/2}\exp(-\beta E_s^{(0)}) \tag{36}$$

where $\omega_0 = (\alpha/M)^{1/2}$.

The free energy can be separated into two parts

$$f_{ph} = (1/\beta)\ln\left(\frac{\beta\xi(1-r)\omega_0}{2\pi b}\right) + \frac{1}{2\beta\xi} \tag{37}$$

and

$$f_{tun} = -\frac{4}{\beta\xi\sqrt{(2\pi)}}(\beta E_s^{(0)})^{-1/2}\exp(-\beta E_s^{(0)}) - \frac{2}{(\beta E_s^{(0)})^2} - \frac{1}{(\beta E_s^{(0)})^3}. \tag{38}$$

Equations (37) and (38) are respectively the phonon and the tunnelling contributions to the free energy. The tunnelling part is due to the presence of kinks and small anharmonic oscillations.

All other thermodynamic quantities can be derived from equation (36). The internal energy U_{int} and the specific heat C_v per particle are respectively given by

$$U_{int} = K_B T + 2\left[\left(\frac{K_B T}{E_s^{(0)}}\right)^2 + \left(\frac{K_B T}{E_s^{(0)}}\right)^3\right] + (E_s^{(0)} - \tfrac{1}{2}K_B T)n_K^{tot} \tag{39}$$

$$\frac{C_v}{K_B} = 1 + \frac{4K_B T}{(E_s^{(0)})^2} + \frac{6(K_B T)^2}{(E_s^{(0)})^3} + \left[\left(\frac{E_s^{(0)}}{K_B T} - \frac{1}{2}\right)^2 - \frac{1}{2}\right]n_K^{tot} \tag{40}$$

where n_K^{tot} is the total density of kinks, which has the form

$$n_K^{tot} = \frac{4}{\xi\sqrt{(2\pi)}}(\beta E_s^{(0)})^{-1/2}\exp(-\beta E_s^{(0)}). \tag{41}$$

The entropy S per particle is

$$\frac{S}{K_B} = 1 - \frac{1}{2\xi} + \frac{4K_BT}{(E_s^{(0)})^2} + \frac{2(K_BT)^2}{(E_s^{(0)})^3} + \ln\left(\frac{2\pi b}{\beta\xi\omega_0(1-r)}\right) + \left(\frac{E_s^{(0)}}{K_BT} + \frac{1}{2}\right) n_K^{tot}. \tag{42}$$

The expressions (36) to (42) give the low-temperature thermodynamic properties of the sine–Gordon system with long-range interaction potential of the Kac–Baker type. Their dependence on the long-range interaction parameter is discussed below.

As it appears from these expressions, and as it is well known since the basic works of Krumhansl and Schrieffer [24] and Currie *et al* [19], the presence of the kink is characterized by the terms containing the kink rest energy $E_s^{(0)}$.

The analysis for a given temperature of equations (39)–(42) as a function of r shows that U_{int}, C_v and n_K^{tot} are decreasing functions of r while the entropy is an increasing function. The decreasing behaviour of the kink density can be understood if we appeal to the fact that an increase of the range of interaction leads to an increase of the kink width. Consequently, compared to the state where the kink width is small (and the number of kinks large), there appears more disorder and the entropy of system increases. It is also seen, as can be expected, that these thermodynamic properties increase with the temperature. Figure 2 shows the variation of the specific heat C_v versus the temperature for different values of the interaction parameter.

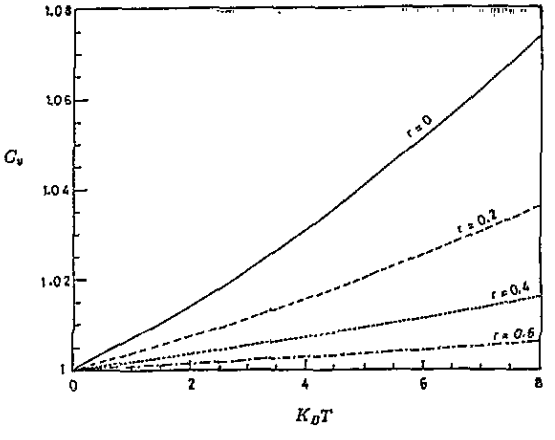

Figure 2. Specific heat versus the temperature for various values of r ($C = 3$, $\alpha = 2$, $M = 1$).

4. Conclusion

In this paper, we have considered the SG model complicated by a long-range interaction potential of Kac–Baker type. The dispersion relations for phonons and an implicit form for topological solitons have been obtained. The width and the energy of the solitons increase

as the range of interaction increases. We have also analysed the thermodynamic properties of the model in the low-temperature regime. For a given temperature, when the range of interaction increases, the specific heat and the internal energy decrease while the entropy increases. Such behaviour is understandable if we appeal to the fact that the increases of the range of interaction lead to the increase or the wide spread of disorder in the system. In the short-range limit ($r = 0$), our results reduce to that of a SG system with nearest-neighbour interactions.

In the dynamical point of view, we have not considered the localized excitations of breather type that exist in the standard SG model. This is because of the mathematical difficulties encountered in the long-range interaction model. Moreover, it would be interesting to study, for various values of interaction parameter r, kink–kink and kink–antikink collisions to find whether or not the solitons obtained in the present paper are transparent. To this aim, numerical experiments, such as those developed in [18] to investigate the properties of solitons in the Peyrard–Remoissenet non-linear deformable substrate potential, should be carried out.

In the thermodynamic domain, our investigations have been limited to the low-temperature regime and classical limit where the pseudo-Schrödinger equation and the associated WKB approximation are valid. The intermediate and high-temperature behaviours (although in this later regime the kinks no longer play a role) are subjects of particular interest, as well as the quantum-statistical mechanics of the long-range interaction models.

Acknowledgments

The authors acknowledge the referees for useful recommendations.

References

[1] Sarker S K and Krumhansl J A 1981 *Phys. Rev.* B **23** 2374
[2] Ishimori Y 1982 *Prog. Theor. Phys.* **68** 402
[3] Pokrovsky V L and Virosztek A 1983 *J. Phys. C: Solid State Phys.* **16** 4513
[4] Remoissenet M and Flytzanis N 1985 *J. Phys. C: Solid State Phys.* **18** 1573
[5] Roseneau Ph 1983 *Phys. Rev.* B **36** 5868
[6] Ferrer R 1989 *Phys. Rev.* B **40** 11 007
[7] Braun O M, Kivshar Y S and Zelenskaya I I 1990 *Phys. Rev.* B **41** 7118
[8] Woafo P, Kofané T C and Bokosah A S 1991 *J. Phys.: Condens. Matter* **3** 2279
[9] Woafo P, Kofané T C and Bokosah A S 1992 *J. Phys.: Condens. Matter* **4** 3389
[10] Tchawoua C, Kofané T C and Bokosah A S 1993 *J. Phys. A: Math. Gen.* **26** 6477
[11] Kittel C 1970 *Introduction à la Physique de l'État Solide* 2nd edn (New York: Wiley) ch 5
[12] Büttner H and Bilz H 1978 *Solitons and Condensed Matter Physics* ed A R Bishop and T Schneider (Berlin: Springer) p 162
[13] Baker G A Jr 1961 *Phys. Rev.* **122** 1477
Kac M and Helfand E 1973 *J. Math. Phys.* **4** 1078
[14] Pnevmatikos St 1983 *CR Acad. Sci. Paris II* **296** 1031
[15] Pnevmatikos St 1984 *Proc. Int. Conf. on Singularities and Dynamical Systems* ed Sp Pnevmatikos (Amsterdam: North-Holland)
[16] Woafo P, Kofané T C and Bokosah A S 1993 *Phys. Rev.* B **48** 10 153
[17] Woafo P, Kenné J R and Kofané T C 1993 *J. Phys.: Condens. Matter* **5** L123
[18] Peyrard M and Remoissenet M 1982 *Phys. Rev.* B **26** 2886
[19] Currie J K, Krumhansl J A, Bishop A R and Trullinger S E 1980 *Phys. Rev.* B **22** 477
[20] Scalapino D J, Sears M and Ferrel R S 1972 *Phys. Rev.* B **26** 3409
[21] Gupta N and Sutherland B 1976 *Phys. Rev.* A **14** 1790

[22] Abramowitz M and Stegun I A 1944 *Handbook of Mathematical Functions* (Washington, DC: National Bureau of Standards)
[23] Schneider T and Stoll E 1980 *Phys. Rev.* B **22** 5317
[24] Krumhansl J A and Schrieffer J R 1975 *Phys. Rev.* B **11** 3535