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Classical statistical mechanics of a sine-Gordon and double sine-Gordon chain with long-range interactions

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Abstract. The formalism developed by Sarker and Krumhansl for the investigation of a ϕ^4 system with long-range interactions of the Kac-Baker type is extended to the study of the thermodynamical properties of a sine-Gordon (SG) and a double sine-Gordon (DSG) chain with long-range interactions. This extension enlarges the class of non-linear systems which can support kink solutions. In the continuum limit we deduce compact analytical expressions for the SG-kink solutions and the DSG-kink solutions as well as for their associated energies. Both the kink solutions and the kink energies depend on the kink width. As the interaction range increases it is found that the kink width and the kink energy increase indefinitely—the kinks disappear. Consequently one can consider the kinks as 'elementary excitations' only in the limit of not too large interaction ranges, when they will destroy long-range order in the system. For this limit we determined the phonon and kink contribution to the free-energy density at low temperatures. For the infinite interaction range limit we found that the two systems studied undergo a second-order phase transition. The critical behaviour is—as expected—similar to that of the ϕ^4 system with long-range interactions.

1. Introduction

It is now well recognised that in many areas of physics it is important to study non-linear equations which possess large-amplitude solitary wave or kink solutions in addition to the small-amplitude modes (phonons, spin waves) characteristic of the linearised equations. Therefore studies concerning the dynamical and thermodynamical properties of kink-bearing systems have been of considerable recent interest, the role which the kinks (solitons) play in the low-temperature thermodynamics being very well established. The investigation of different systems subjected to non-linear substrate potentials like the ϕ^4, double quadratic (DQ), sine-Gordon (SG) (Krumhansl and Schrieffer 1975, Gupta and Sutherland 1976, Guyer and Miller 1976, DeLeonardis and Trullinger 1979, Trullinger and DeLeonardis 1979, Bishop *et al* 1980, Currie *et al* 1980) as well as double sine-Gordon (DSG) (Condat *et al* 1983, DeLeonardis and Trullinger 1983, Leung 1982, 1983, Pandit *et al* 1983a, b, Giachetti *et al* 1984) or other doubly periodic parametrised symmetric and asymmetric potentials (Remoissenet and Peyrard 1984, Croitoru 1987) has been limited to one-dimensional models and nearest-neighbour (NN) interactions between the atoms of the chain. These limitations are essentially due to the mathematical difficulties encountered in investigating models of higher dimensions or by taking into account, for 1D models, interactions of longer than NN range. Recently, there have been reported studies of systems which include next-

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nearest-neighbour (NNN) interactions (Pnevmatikos 1984, Flytzanis *et al* 1987), and even use long-range interaction potentials of the Lennard-Jones type (Ishimori 1982). Other interesting results have been obtained by investigating a non-linear system of the ϕ^4 type (Sarker and Krumhansl 1981) and an anharmonic chain (Remoissenet and Flytzanis 1985) with a long-range Kac-Baker interaction potential. While Sarker and Krumhansl (1981) studied the effect of the kink solutions on the thermodynamics of the ϕ^4 system, Remoissenet and Flytzanis (1985) concentrated solely on the dynamics of the anharmonic chain with long-range interactions.

The purpose of this paper is to study the properties of sine-Gordon and double sine-Gordon systems with long-range Kac-Baker interaction potentials, in which the interaction between the particles falls off exponentially as $\exp(-\gamma x)$ as their separation, x, increases.

In § 2 we present the Hamiltonian of the systems under study and, paralleling the procedure developed in Sarker and Krumhansl (1981), we briefly sketch the derivation of the associated equation of motion. Subsequently, we determine in closed form its small-amplitude (phonon) and large-amplitude (kink) solutions in the continuum limit. We also succeed in deriving compact expressions for the kink energies. In § 3 we treat the classical statistical mechanics of the two chosen systems in two limiting cases: (i) $\gamma \gg 1$, in which the interaction range does not go far beyond the nearest neighbours; and (ii) $\gamma \to 0$, the infinite interaction range limit. The method adopted to perform these studies is that developed in Sarker and Krumhansl (1981) and is based on a transformation which converts the partition function into a functional integral in which the effective interaction couples only NN. Section 4 summarises the main results.

2. Excitations of the SG and DSG systems

Let us consider a one-dimensional system of N atoms governed by the Hamiltonian

$$H = \sum_i A\left(\tfrac{1}{2}\dot{\phi}_i^2 + \tfrac{1}{2}c_0^2 \frac{1-r}{2r} \sum_{j \neq i} r^{|i-j|}(\phi_i - \phi_j)^2 + \omega_0^2 V(\phi_i)\right). \tag{1}$$

Here ϕ_i represents the one-component dimensionless scalar field, A is a constant which sets the energy scale, and c_0 and ω_0 are respectively a characteristic velocity and a characteristic frequency. The lattice constant l and the mass m of the interacting particles are taken to be unity. The atoms labelled by the indices i, j are assumed to interact via a pair potential of the Kac-Baker form

$$V_{ij} = Ac_0^2 \frac{1-r}{2r} r^{|i-j|} \tag{2}$$

where $r = \exp(-\gamma)$, and γ^{-1} essentially defines the interaction range. There are two requirements which one has to impose on the second term of (1). First, in the limit $r \to 0$, $\gamma \to \infty$, the Hamiltonian (1) has to describe a non-linear system with NN interactions. The presence of the factor r^{-1} ensures the fulfilment of this requirement. Secondly, for any value taken by r in the interval $(0, 1)$, the thermodynamic limit has to exist, i.e. the total interaction potential experienced by an atom of the chain from all the other atoms has to be finite. Due to the introduction of the factor $(1-r)$ this condition will also be fulfilled.

The non-linear potential $V(\phi)$ which appears in (1) will be considered to be of the following two forms:

$$\text{SG potential} \qquad V(\phi) = 1 + \cos\phi \tag{3a}$$

$$\text{DSG potential} \qquad V(\phi) = \frac{2}{1-\alpha^2}(\cos\tfrac{1}{2}\phi - \alpha)^2 \tag{3b}$$

where the parameter α is confined to the interval $0 \leqslant \alpha < 1$. For $\alpha = 0$, equation (3*b*) transforms into (3*a*). The potentials (3*a*) and (3*b*) possess (Condat *et al* 1983, DeLeonardis and Trullinger 1983) the following symmetry and periodicity properties:

$$V(\phi) = V(-\phi)$$

$$V(\phi) = V(\phi + p)$$

with $p = 2\pi$ (SG) and $p = 4\pi$ (DSG).

While the potential (3*a*) is characterised by potential barriers of equal height and potential wells of equal curvature, the DSG potential (3*b*) possesses potential barriers of two different heights, but two adjacent minima have the same shape. For the SG potential the local minima are found at

$$\phi = (2n+1)\pi \qquad n = 0, \pm 1, \pm 2, \ldots \tag{4a}$$

while the local maxima are found at

$$\phi = 2\pi n \qquad n = 0, \pm 1, \pm 2, \ldots. \tag{4b}$$

We note that for $\phi = 2\pi n$, the potential takes the constant value

$$V(\phi = 2\pi n) = 2 \tag{5a}$$

and for $\phi = (2n+1)\pi$ we have

$$V(\phi = (2n+1)\pi) = 0. \tag{5b}$$

At the local minima the second derivative $V''(\phi)$ is normalised to unity.

In the case of the DSG potential (3*b*) the local minima are situated at

$$\phi = \pm\phi_1 + 4\pi n \qquad n = 0, \pm, \pm 2, \ldots \tag{6a}$$

where

$$\phi_1 = 2\cos^{-1}\alpha \tag{7}$$

and the local maxima are found at

$$\phi = 4\pi n \qquad n = 0, \pm 1, \pm 2, \ldots \tag{6b}$$

and at

$$\phi = 2\pi(2n+1) \qquad n = 0, \pm 1, \pm 2, \ldots. \tag{6c}$$

At the points (6*b*) and (6*c*) the potential barriers are of the following heights:

$$V(\phi = 4\pi n) = 2\frac{1-\alpha}{1+\alpha} \qquad \text{(low barrier)} \tag{8a}$$

$$V(\phi = 2\pi(2n+1)) = 2\frac{1+\alpha}{1-\alpha} \qquad \text{(high barrier)} \tag{8b}$$

and for $\phi = \pm\phi_1 + 4\pi n$, $V(\phi) = 0$. The second derivative $V''(\phi)$ corresponding to the local minima (6*a*) is normalised to unity. This property does not imply that the curvature of the DSG potential wells does not depend on the parameter α. Indeed, discarding the denominator $(1-\alpha^2)$ in (3*b*) one gets

$$V''(\phi = \pm\phi_1 + 4\pi n) = 1 - \alpha^2. \tag{9}$$

Consequently for $\alpha \to 1$, the bottom of the potential wells becomes very flat. In the following we will always restrict our attention to very small values of α.

The equation of motion associated with (1) can be written

$$\ddot{\phi}_i + c_0^2 \frac{1-r}{r} \sum_{j \neq i} r^{|i-j|}(\phi_i - \phi_j) + \omega_0^2 \frac{dV}{d\phi_i} = 0. \tag{10}$$

The main problem now is to reduce (10) into an equivalent 'nearest-neighbour' problem. This is achieved by introducing the quantity (Sarker and Krumhansl 1981)

$$L_i = c_0^2 \frac{1-r}{r} \sum_{j \neq i} r^{|i-j|}\phi_j. \tag{11}$$

Substitution of (11) into (10) gives

$$L_i = \ddot{\phi}_i + 2c_0^2\phi_i + \omega_0^2 \frac{dV}{d\phi_i}. \tag{12}$$

Here we have used the relation

$$c_0^2 \frac{1-r}{r} \sum_{j \neq i} r^{|i-j|} = 2c_0^2. \tag{13}$$

Now,

$$L_{i+1} + L_{i-1} = c_0^2 \frac{1-r}{r}\left((r + r^{-1}) \sum_{j \neq i} r^{|i-j|}\phi_j + 2r\phi_i - \phi_{i+1} - \phi_{i-1}\right) \tag{14}$$

but by use of (11) this becomes

$$L_{i+1} + L_{i-1} = (r + r^{-1})L_i + c_0^2 \frac{1-r}{r}(2r\phi_i - \phi_{i+1} - \phi_{i-1}). \tag{14'}$$

We remark that only 'nearest-neighbour' quantities are involved in (14'). Assuming (Sarker and Krumhansl 1981) that the lattice constant is much smaller than the width of a kink (than the wavelength of the phonons) the quantities L_{i+1} (L_{i-1}) and the field variables ϕ_{i+1} (ϕ_{i-1}) can be expanded in Taylor series about the lattice position labelled by *i*. Then, in this limit—the continuum limit—all quantities which appear in (14') can be assumed to become continuous functions of the position variable *x*. Therefore we may write

$$\begin{aligned} &\phi_i \to \phi(x) \qquad L_i \to L(x) \\ &\phi_{i+1} + \phi_{i-1} \simeq 2\phi(x) + \phi''(x) \qquad L_{i+1} + L_{i-1} \simeq 2L(x) + L''(x) \end{aligned} \tag{15}$$

and by also taking account of (12) we obtain the final form of the equation of motion

$$\phi_{tt} - c^2(r)\phi_{xx} = -\omega_0^2 V' + f(r)[\omega_0^2(V'_{xx} + \tfrac{1}{12}V'_{xxxx}) + \phi_{tt,xx}] + \tfrac{1}{12}c^2(r)\phi_{xxxx} \tag{16}$$

where

$$V' = \frac{dV}{d\phi} \qquad \phi_{tt} = \frac{d^2\phi_x}{dt^2} \qquad \phi_{xx} = \frac{d^2\phi_x}{dx^2} \qquad V'_{xx} = \frac{d^2V'}{dx^2}$$

and so on, and

$$c^2(r)=\frac{1+r}{(1-r)^2}c_0^2 \qquad f(r)=\frac{r}{(1-r)^2}. \tag{17}$$

While $c(r)$ represents a velocity dependent on the parameter r, $f(r)$ is a factor which characterises the dispersion terms involved in (16). For $r=0$, (16) recovers the well known equation of motion of a non-linear system governed by NN interactions.

In the following we shall show that for the two non-linear substrate potentials (3*a*) and (3*b*), equation (16) supports kink solutions as well as small-amplitude oscillations. It is our aim to derive their analytic expressions together with the kink energies.

2.1. *Small-amplitude solutions*

By discarding in (16) the fourth-order derivative with respect to the variable x, we look for small-amplitude solutions both about the top of the potential barriers and about the bottom of the potential wells.

2.1.1. Oscillations about ϕ corresponding to the top of the potential barriers. In the SG case we look for solutions of the form

$$\exp[\mathrm{i}(qx-\omega t)]$$

and in the DSG case for solutions of the form

$$\phi-2\pi n\sim\exp[\mathrm{i}(qx-\omega t)] \qquad n=1,2,\ldots.$$

For both non-linear systems (3*a*) and (3*b*), the dispersion relation is of the same form, namely

$$\omega_q^2=-\omega_0^2+\frac{c^2(r)q^2}{1+f(r)q^2} \tag{18}$$

where q represents the wavevector, and $c(r)$ and $f(r)$ are defined in (17). Here the wavevector q has to satisfy the inequality

$$q^2>\frac{\omega_0^2}{c^2(r)-f(r)\omega_0^2} \tag{19}$$

otherwise the frequency ω_q^2 becomes negative.

The energy of these phonons is given by

$$\varepsilon=A\omega_0^2L+\hbar\omega \tag{20}$$

where L is the length of the chain. The first term in (20) is due to the contribution of all atoms contained in the chain.

2.1.2. Oscillations about the bottom of the potential wells. The solutions we look for are of the form

$$\phi-\phi_{\mathrm{m}}\sim\exp[\mathrm{i}(qx-\omega t)]$$

with $\phi_{\mathrm{m}}=\pi$ in the SG case and $\phi_{\mathrm{m}}=\phi_{1,2}$ in the DSG case.

Again, for both non-linear potentials (3*a*) and (3*b*) we obtain the same dispersion law

$$\omega_q^2=\omega_0^2+\frac{c^2(r)q^2}{1+f(r)q^2}. \tag{21}$$

In this case there does not exist any restriction which has to be satisfied by the wavevector q.

As expected, for $r=0$ (21) is the well known dispersion relation corresponding to a sine-Gordon system with single or double periodicity and with NN interactions:

$$\omega_q^2=\omega_0^2+\omega_0^2 q^2.$$

2.2. *Kink solutions*

In order to obtain an equation which, with properly chosen boundary conditions, yields kink solutions we neglect in (16) all derivatives of higher than second order. This step is in the spirit of the continuum approximation, and moreover all neglected terms will disappear from (16) for $v=0$ and/or $r=0$. Thus we have to look for solutions of the equation

$$(c^2(r)-v^2)\phi_{zz}-\omega_0^2 V'+f(r)\omega_0^2 V'_{zz}=0 \tag{22}$$

where $z=x-vt$, v being the velocity of the moving kink. If we introduce the quantities

$$\xi^2=(c^2(r)-v^2)/\omega_0^2 \tag{23a}$$

$$\sigma=f(r)/\xi \tag{23b}$$

and a new variable $y=z/\xi$, then (22) transforms into

$$\mathrm{d}^2\phi/\mathrm{d}y^2+\sigma(V')_{yy}-V'=0 \tag{22'}$$

which, for $r=0$, is the well known equation of motion of a non-linear system with NN interactions.

For the non-linear substrate potentials (3a) and (3b), equation (22') supports kink solutions which have to satisfy boundary conditions.

(i) In the SG case the conditions are

$$\phi(y)=\pi \qquad \mathrm{d}\phi/\mathrm{d}y=0 \qquad \text{for } y=\pm\infty. \tag{24}$$

(ii) For the DSG chain there is a set of conditions for the first kink solution

$$\phi=\phi_1 \qquad \mathrm{d}\phi/\mathrm{d}y=0 \qquad \text{for } y=\pm\infty \tag{25a}$$

and another set for the second kink solution

$$\phi=4\pi-\phi_1=\phi_2 \qquad \mathrm{d}\phi/\mathrm{d}y=0 \qquad \text{for } y=\pm\infty. \tag{25b}$$

Here ϕ_1 is defined in (7). While for the SG system there exists a single kink solution, for the DSG system we have two different kink solutions. The type-I kink evolves the system from one well to the adjacent one over the type-I barrier (the small barrier (8a)), while the type-II kink describes the evolution of the system over the type-II barrier (the high barrier (8b)). With the above stated boundary conditions, equation (22') can be integrated for the two models under consisideration, to give

SG system
$$\frac{\mathrm{d}\phi}{\mathrm{d}y}=\sqrt{2V}\frac{\sqrt{1+\sigma\sin^2\frac{1}{2}\phi}}{1+\sigma V''} \tag{26a}$$

DSG system
$$\frac{\mathrm{d}\phi}{\mathrm{d}y}=\frac{\sqrt{2V}}{\sqrt{1-\alpha^2}}\frac{\sqrt{1-\alpha^2+\sigma\sin^2\frac{1}{2}\phi}}{1+\sigma V''} \tag{26b}$$

Obviously the potential (3*a*) is involved in (26*a*), whereas the potential in (26*b*) is (3*b*). The integration of (26*a*) and (26*b*) yields the kink solutions which, especially for the DSG model, are rather complicated expressions.

For the SG system this kink solution is

$$\pm y = \frac{\sqrt{1+\sigma}}{2} \ln\left(\frac{\sqrt{1+\sigma\sin^2\frac{1}{2}\phi}+\sqrt{1+\sigma}\sin\frac{1}{2}\phi}{\sqrt{1+\sigma\sin^2\frac{1}{2}\phi}-\sqrt{1+\sigma}\sin\frac{1}{2}\phi}\right) - 2\sqrt{\sigma}\ln\left(\sqrt{1+\sigma\sin^2\tfrac{1}{2}\phi}+\sqrt{\sigma}\sin\tfrac{1}{2}\phi\right). \tag{27}$$

For the DSG system the kink solutions are

$$\begin{aligned}\pm y^{(\mathrm{I})} \simeq \sqrt{1-\alpha^2+\sigma}\Bigg[& -\frac{1}{\alpha}(\Pi-\tilde{\Pi}) - \frac{\sqrt{1-\alpha^2+\sigma}}{2(1-\alpha^2)\sqrt{1+\sigma}} \\ & \times \ln\left(\frac{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\phi}}-\sqrt{1+\sigma}\sin\tilde{\phi}}{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\phi}}+\sqrt{1+\sigma}\sin\tilde{\phi}}\right)\Bigg] \\ & - 2\sqrt{\sigma}\ln\left(\frac{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\phi}}+\sqrt{\sigma}\sin\tilde{\phi}}{\sqrt{1-\alpha^2}}\right) - \frac{\sigma\alpha}{\sqrt{1-\alpha^2+\sigma}}(F-\tilde{F}-\Pi+\tilde{\Pi}) \\ & + \frac{\alpha\sigma^2}{2(1-\alpha^2)\sqrt{1+\sigma}}\ln\left(\frac{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\phi}}-\sqrt{1+\sigma}\sin\tilde{\phi}}{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\phi}}+\sqrt{1+\sigma}\sin\tilde{\phi}}\right)\end{aligned} \tag{28a}$$

$$\begin{aligned}\pm y^{(\mathrm{II})} \simeq \sqrt{1-\alpha^2+\sigma}\Bigg[& -\frac{1}{\alpha}(\Pi-\tilde{\tilde{\Pi}}) + \frac{\sqrt{1-\alpha^2+\sigma}}{2(1-\alpha^2)\sqrt{1+\sigma}} \\ & \times \ln\left(\frac{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\tilde{\phi}}}-\sqrt{1+\sigma}\sin\tilde{\tilde{\phi}}}{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\tilde{\phi}}}+\sqrt{1+\sigma}\sin\tilde{\tilde{\phi}}}\right)\Bigg] \\ & + 2\sqrt{\sigma}\ln\left(\frac{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\tilde{\phi}}}+\sqrt{\sigma}\sin\tilde{\tilde{\phi}}}{\sqrt{1-\alpha^2}}\right) \\ & - \frac{\sigma\alpha}{\sqrt{1-\alpha^2+\sigma}}(F-\tilde{\tilde{F}}-\Pi+\tilde{\tilde{\Pi}}) \\ & - \frac{\sigma\alpha^2}{2(1-\alpha^2)\sqrt{1+\sigma}}\ln\left(\frac{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\tilde{\phi}}}-\sqrt{1+\sigma}\sin\tilde{\tilde{\phi}}}{\sqrt{1-\alpha^2+\sigma\sin^2\tilde{\tilde{\phi}}}+\sqrt{1+\sigma}\sin\tilde{\tilde{\phi}}}\right).\end{aligned} \tag{28b}$$

Here the superscripts I and II label the two different kink solutions, and for the field variable we have introduced the notation

$$\tilde{\phi} = \tfrac{1}{2}\phi - 2\pi n \qquad \tilde{\tilde{\phi}} = \tfrac{1}{2}\phi - 2\pi(n+\tfrac{1}{2}) \qquad n = 0, \pm 1, \pm 2, \ldots .$$

The various elliptical integrals of the first and third kinds are defined as follows:

$$\begin{aligned} & F = F(\tfrac{1}{2}\pi, k) \qquad \tilde{F} = F(\tfrac{1}{2}\pi - \tilde{\phi}, k) \qquad \tilde{\tilde{F}} = F(\tfrac{1}{2}\pi - \tilde{\tilde{\phi}}, k) \\ & \Pi = \Pi(\tfrac{1}{2}\pi, -1/\alpha^2, k) \qquad \tilde{\Pi} = \Pi(\tfrac{1}{2}\pi - \tilde{\phi}, -1/\alpha^2, k) \qquad \tilde{\tilde{\Pi}} = \Pi(\tfrac{1}{2}\pi - \tilde{\tilde{\phi}}, -1/\alpha^2, k)\end{aligned} \tag{29}$$

and

$$k^2 = \sigma/(1-\alpha^2+\sigma). \tag{30}$$

From (28*a*) and (28*b*) it follows immediately that for $\alpha = 0$, $y^{(\mathrm{I})} = y^{(\mathrm{II})} = y$ becomes the SG kink solution (27) and for $\sigma = 0$, we recover the two kink solutions of the DSG

chain with NN interactions (DeLeonardis and Trullinger 1983). Moreover, for $\alpha = 0$ and $\sigma = 0$ we get

$$\phi = 4\tan^{-1}\left[\tanh\left(\pm\frac{x-vt}{2d}\right)\right]. \tag{31}$$

In equations (27), (28*a*), (28*b*) and (31) the positive (negative) sign corresponds to the kink (antikink) solution. We conclude this subsection with some comments both with respect to the two parameters σ, ξ and to the kink solutions. The σ term in the equation of motion (22′) breaks the Lorentz invariance of the short-range problem. The parameter σ is always small, and for $r \to 1$ it approaches its limiting value $\omega_0^2/2c_0^2 = 1/2d$, where d measures the width of a kink corresponding to a nearest-neighbour interaction problem. The quantity ξ defined by (23*a*) and involved in the kink solutions via the variable y, has the dimension of length, which for a static kink ($v = 0$) becomes $\xi_s = c(r)/\omega_0$. It is a measure of the width of a kink, and diverges as $(1-r)^{-1}$. Thus the kinks are of finite width, only for small values of r while for $r \to 1$ they slowly disappear; the width becomes infinite, and in accordance with (27), (28*a*) and (28*b*), the field variable $\phi = 2\pi n$ ($n = 0, \pm 1, \pm 2, \ldots$) for all values of x. This means that the particles cease to jump from one well to the adjacent one; they remain sitting on the top of the potential barriers, both in the SG and DSG systems.

2.3. The kink energy

In order to derive compact expressions for the energy of the SG kink as well as of the two DSG kinks, we start from that part of the Hamiltonian (1) which includes all the potential terms:

$$E_p = \sum_i A\left(\omega_0^2 V(\phi_i) + \tfrac{1}{2}c_0^2 \frac{1-r}{2r} \sum_{j \neq i} r^{|i-j|}(\phi_i - \phi_j)^2\right). \tag{32}$$

Taking into account (11)–(13) and adopting the continuum limit, (32) transforms into

$$E_p = A\left(\int_{-\infty}^{+\infty} dy\, V[\phi_k(y)] - \frac{\xi\omega_0^2}{2}\int_{-\infty}^{+\infty} dy\, \phi_k(y)\frac{dV}{d\phi_k} - \frac{v^2}{2\xi}\int_{-\infty}^{+\infty} dy\, \phi_k(y)\frac{d^2\phi_k}{dy^2}\right) \tag{33}$$

where $y = (x - vt)/\xi$ and $\phi_k(y)$ represents a kink solution, being given either by (27) or (28*a*) and (28*b*). Remarking that $d\phi = \phi_y\, dy$, the three intregrals which appear in (33) can be written as

$$E_1 = 2A\xi\omega_0^2 \int_0^{\phi_{min}} d\phi \frac{V(\phi)}{\phi_y} \tag{34a}$$

$$E_2 = A\xi\omega_0^2 \int_0^{\phi_{min}} d\phi \left(\frac{V(\phi)}{\phi_y} - \frac{V(\phi)}{\phi_y}\frac{\phi}{\phi_y}\frac{d\phi_y}{d\phi}\right) \tag{34b}$$

$$E_3 = \frac{Av^2}{\xi}\int_0^{\phi_{min}} d\phi\, \phi_y = -\frac{Av^2}{\xi}\int dy\, \phi_y^2 = E_c. \tag{34c}$$

Here ϕ_y is given by (26*a*) and (26*b*), E_c represents the kinetic energy and ϕ_{min} the value of ϕ taken at the bottom of the well. In the SG case $\phi_{min} = \pi$, and in the DSG case, there exist two minima within a period of the potential, namely at $\phi = \phi_1$ and

at $\phi = 4\pi - \phi_1 = \phi_2$. Performing the integrations we obtain for the SG system:

$$E_p = E_1 + E_2 = 2A\xi\omega_0^2\left[3\sqrt{1+\sigma} - \left(2\sqrt{\sigma} - \frac{1}{\sqrt{\sigma}}\right)\tanh^{-1}\sqrt{\frac{\sigma}{1+\sigma}}\right] \tag{35a}$$

$$E_3 = \frac{2Av^2}{\xi}\frac{1}{\sqrt{\sigma}}\left(\sqrt{\frac{1+\sigma}{1-\sigma}}\tan^{-1}\sqrt{\frac{\sigma}{1+\sigma}} + \tanh^{-1}\sqrt{\frac{\sigma}{1+\sigma}}\right) \tag{35b}$$

and for the DSG system:

$$E_p^{(I)} = E_1^{(I)} + E_2^{(I)} = 2A\xi\omega_0^2\left[3\sqrt{1+\sigma} - \left(2\frac{(1+\alpha^2)}{1-\alpha^2}\sqrt{\sigma} - \frac{1}{\sqrt{\sigma}}\right)\tanh^{-1}\sqrt{\frac{\sigma}{1+\sigma}} + 2\alpha\frac{\sqrt{1-\alpha^2+\sigma}}{1-\alpha^2}(\tilde{F}-F) - 4\alpha\frac{\sqrt{1-\alpha^2+\sigma}}{1-\alpha^2}(\tilde{E}-E)\right] \tag{36a}$$

$$E_3^{(I)} = \frac{4Av^2}{\xi}\frac{1}{\sqrt{\sigma}}\frac{1}{\sqrt{8+\alpha^2k^2}}(I_a - I_b) \tag{36b}$$

and

$$E_p^{(II)} = 2A\xi\omega_0^2\left[3\sqrt{1+\sigma} - \left(2\frac{(1+\alpha^2)}{1-\alpha^2}\sqrt{\sigma} - \frac{1}{\sqrt{\sigma}}\right)\tanh^{-1}\sqrt{\frac{\sigma}{1+\sigma}} - 2\alpha\frac{\sqrt{1-\alpha^2+\sigma}}{1-\alpha^2}(\tilde{\tilde{F}}-F) + 4\alpha\frac{\sqrt{1-\alpha^2+\sigma}}{1-\alpha^2}(\tilde{\tilde{E}}-E)\right] \tag{37a}$$

$$E_3^{(II)} = \frac{4Av^2}{\xi}\frac{1}{\sqrt{\sigma}}\frac{1}{\sqrt{8+\alpha^2k^2}}(I_{\tilde{a}} - I_{\tilde{b}}). \tag{37b}$$

Here the quantities I_a, I_b, $I_{\tilde{a}}$ and $I_{\tilde{b}}$ are defined by

$$I_c = (1-c^2k^2)(c-\alpha)\left(\frac{-1}{c}(\Pi_c - \tilde{\Pi}_c)\right) - \frac{1}{2\sqrt{1-c^2}\sqrt{1-c^2k^2}}\ln\left(\frac{\sqrt{1-c^2}\sqrt{1-k^2\alpha^2} - \sqrt{1-\alpha^2}\sqrt{1-k^2c^2}}{\sqrt{1-c^2}\sqrt{1-k^2\alpha^2} + \sqrt{1-\alpha^2}\sqrt{1-k^2c^2}}\right) + k(c-\alpha)\ln\left(\frac{\sqrt{1-k^2}}{k\sqrt{1-\alpha^2}+\sqrt{1-k^2\alpha^2}}\right) - k^2c(c-\alpha)(F-\tilde{F}) + (E-\tilde{E}) \tag{38a}$$

$$I_{\tilde{c}} = (\alpha+\tilde{c})(1-\tilde{c}^2k^2)\left(-\frac{1}{\tilde{c}}(\tilde{\tilde{\Pi}}_{\tilde{c}} - \Pi_{\tilde{c}})\right) + \frac{1}{2\sqrt{1-\tilde{c}^2}\sqrt{1-\tilde{c}^2k^2}}\ln\left(\frac{\sqrt{1-\tilde{c}^2}\sqrt{1-k^2\alpha^2} + \sqrt{1-\alpha^2}\sqrt{1-k^2\tilde{c}^2}}{\sqrt{1-\tilde{c}^2}\sqrt{1-k^2\alpha^2} - \sqrt{1-\alpha^2}\sqrt{1-k^2\tilde{c}^2}}\right) + k(\alpha+\tilde{c})\ln\left(\frac{\sqrt{1-k^2\alpha^2} - k\sqrt{1-\alpha^2}}{\sqrt{1-k^2}}\right) - k^2\tilde{c}(\alpha+\tilde{c})(\tilde{\tilde{F}}-F) + (\tilde{\tilde{E}}-E) \tag{38b}$$

where c is taken to represent either a or b, while $\tilde{c}$ represents either $\tilde{a}$ or $\tilde{b}$. These latter parameters are defined by

$$a = \tfrac{1}{4}[\alpha + (1/k)\sqrt{8+\alpha^2k^2}] \qquad b = \tfrac{1}{4}[\alpha - (1/k)\sqrt{8+\alpha^2k^2}] \tag{39a}$$

$$\tilde{a} = -\tfrac{1}{4}[\alpha - (1/k)\sqrt{8+\alpha^2k^2}] \qquad \tilde{b} = -\tfrac{1}{4}[\alpha + (1/k)\sqrt{8+\alpha^2k^2}] \tag{39b}$$

and k is given by (30). The elliptical integrals of first, second and third kinds involved in relations (36a), (37a), (38a) and (38b) are defined in the following way:

$$F = F(\tfrac{1}{2}\pi, k) \qquad \tilde{F} = F(\tfrac{1}{2}\pi - \tfrac{1}{2}\phi_1, k) \qquad \tilde{\tilde{F}} = F(\tfrac{3}{2}\pi - \tfrac{1}{2}\phi_1, k)$$

$$E = E(\tfrac{1}{2}\pi, k) \qquad \tilde{E} = E(\tfrac{1}{2}\pi - \tfrac{1}{2}\phi_1, k) \qquad \tilde{\tilde{E}} = E(\tfrac{3}{2}\pi - \tfrac{1}{2}\phi_1, k) \tag{40}$$

$$\Pi_c = \Pi(\tfrac{1}{2}\pi, -1/c^2, k) \qquad \tilde{\Pi}_c = \Pi(\tfrac{1}{2}\pi - \tfrac{1}{2}\phi_1, -1/c^2, k) \qquad \tilde{\tilde{\Pi}}_c = \Pi(\tfrac{3}{2}\pi - \tfrac{1}{2}\phi_1, -1/c^2, k)$$

and $\Pi_{\tilde{c}}$, $\tilde{\Pi}_{\tilde{c}}$, $\tilde{\tilde{\Pi}}_{\tilde{c}}$ are obtained from Π_c, $\tilde{\Pi}_c$, $\tilde{\tilde{\Pi}}_c$ by replacing c by $\tilde{c}$.

In the limit $\alpha = 0$ equations (36a) and (37a) transform into (35a). For $r = 0$ ($\sigma = 0$), we recover the well known results of either the SG or DSG systems with NN interactions. Since the kink energies (35a), (36a) and (37a) are proportional to ξ, they will increase indefinitely as $r \to 1$. Therefore only for small values of r will the kink energies associated with the SG and DSG kinks (27), (28a) and (28b) be finite, and in this case the kinks can be regarded as 'low-energy excitations', which in the low-temperature limit will show up in the free energy of the systems under study. As $r \to 1$ the kink activation energy becomes indefinitely large. These kinks of infinite width and very high activation energy will not determine the low-temperature thermodynamical properties of the systems under study. Though the kink solutions (27), (28a) and (28b) and the kink energies (35)–(38) are quite different from those deduced for the ϕ^4 system with long-range interactions (Sarker and Krumhansl 1981), as expected, their qualitative properties are similar.

3. Statistical mechanics

In this section we present our results concerning the thermodynamical properties of the SG and DSG chain with long-range interactions, with the objective of identifying kink contributions to the free energy in the limit of small r and also to demonstrate the existence of a second-order phase transition in the van der Waals limit $r \to 1$. These two objectives will be achieved via the determination of the partition functions of the systems under consideration.

The classical partition function, for N interacting particles, governed by the Hamiltonian (1), is given by

$$Z = \left(\frac{A}{h}\right)^N \int \prod_{i=1}^{N} \mathrm{d}\dot{\phi}_i \int \prod_{i=1}^{N} \mathrm{d}\phi_i \exp(-\beta H) \tag{41}$$

and factorises into the configurational and kinetic parts

$$Z = Z_{\dot{\phi}} Z_{\phi} \tag{42}$$

where

$$Z_{\dot{\phi}} = (2\pi A/\beta h^2)^{N/2} \tag{43a}$$

and

$$Z_{\phi} = \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \left(\prod_i \mathrm{d}\phi_i \exp[-\beta w(\phi)] \right) \exp\left(A\beta c_0^2 \frac{(1-r)}{r} \sum_{j>i} \phi_i \phi_j r^{|i-j|} \right) \tag{43b}$$

with

$$W(\phi) = A[\omega_0^2 V(\phi) + c_0^2 \phi^2]. \tag{44}$$

Here $\beta = (k_B T)^{-1}$, k_B being the Boltzmann constant, and $V(\phi)$ is given by (3*a*) and (3*b*). The principal task consists in the evaluation of Z_ϕ in a closed form. For the Kac-Baker potential (2) the functional integral for Z_ϕ can be transformed into an equivalent NN problem, and moreover, as has been shown by Sarker and Krumhansl (1981), this NN problem not only reduces to the integral equation of Krumhansl and Schieffer (1975) in the limit $r = 0$, but is applicable to any type of field variables and for arbitrary local interactions $W(\phi)$. In this equivalent NN formulation, the partition function Z_ϕ takes the form

$$Z_\phi = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} \prod_{i=1}^{N} \mathrm{d}u_i \left(\prod_{i=1}^{N-1} G(u_i, u_{i+1}) \right) F(u_N). \tag{45}$$

Here

$$G(u, u') = \int_{-\infty}^{+\infty} \mathrm{d}\phi \, \exp[-\beta W(\phi) + \beta A c_0^2 (1-r)\phi u'] \delta(u - \phi - u'r) \tag{46a}$$

$$F(u) = \int_{-\infty}^{+\infty} \mathrm{d}\phi \, \exp[-\beta W(\phi)] \delta(u - \phi) = \exp[-\beta W(u)] \tag{46b}$$

and the variables $\{u\}$ are defined as

$$u_i = \sum_{j=1}^{N} r^{j-i} \phi_j \tag{47}$$

and satisfy the recursion relations

$$u_j = \phi_i + r u_{j+1} \qquad j = 1, 2, \dots, N-1 \tag{48a}$$

$$u_N = \phi_N. \tag{48b}$$

The δ function involved in (46*a*) and (46*b*) ensures that the integrations over the auxiliary variables u_i are restricted by (48*a*) and (46*b*). As it stands, (45) can be regarded as a repeated operation of an integral operator, the eigenvalues of which are given by

$$\int_{-\infty}^{+\infty} \mathrm{d}u_{i+1} \, G(u_i, u_{i+1}) \psi_n(u_{i+1}) = \lambda_n \psi_n(u_i) \tag{49a}$$

$$\int_{-\infty}^{+\infty} \mathrm{d}u_i \, \zeta_n(u_i) G(u_i, u_{i+1}) = \lambda_n \zeta_n(u_{i+1}). \tag{49b}$$

Here ψ_n and ζ_n are the right and left eigenfunctions of the asymmetric integral operator, satisfying the normalisation relation

$$\int_{-\infty}^{+\infty} \mathrm{d}u \, \psi_m(u) \zeta_n(u) = \delta_{mn}. \tag{50}$$

For the determination of the eigenvalues one can use either (49*a*) or (49*b*). Since for the systems under study $W(u) = W(-u)$, the asymmetric kernel G has a definite parity, $G(u, u') = G(-u, -u')$. Then the eigenfunctions are either even or odd. For even eigenfunctions (49*b*) reduces to Baker's functional equation for the Ising model (Baker 1961) and also to that derived for the Ising and Potts models by Viswanathan and Meyer (1977) who showed that the eigenvalues are real and that the largest one is positive. Therefore in the following we shall use (49*b*).

In the thermodynamic limit ($L\to\infty$, $N\to\infty$, with L/N constant) the configurational part of the partition function Z_ϕ is dominated by the largest eigenvalue λ_0, and the free energy per unit length ($F=-(1/\beta L)\ln Z$, where $L=N$, because we have assumed the lattice constant $l=1$) becomes

$$F=-\frac{1}{2\beta}\ln\frac{2\pi A}{\beta h^2}-\ln\lambda_0. \tag{51}$$

3.1. Low-temperature properties in the limit of small r

As shown in § 2, for small values of the parameter r, the width of the kink solutions (27), (28a) and (28b) is finite, and the kink activation energies (35a), (36a) and (37a) are also finite quantities. Then, in the low-temperature limit one can expect a contribution of these kinks to the free energy of the systems under study. In this case, under some restrictive conditions, the integral equation (49b) can be converted into a pseudo-Schrödinger equation which depends on a large parameter. In order to determine the eigenspectrum of this equation one can make use of asymptotic methods (Croitoru *et al* 1984, Croitoru 1987) known from the theory of second-order differential equations which depend on a large parameter (Nayfeh-Hasan 1973). To perform this programme we start by writing (49b) in a more explicit form

$$\int \mathrm{d}u' \exp[-\beta W(u'-ru)+Ac_0^2\beta(1-r)(u'-ru)u]\zeta(u')=\lambda\zeta(u) \tag{52}$$

where

$$\beta W(u'-ru)=\kappa[V(u'-ru)+d^2(u'-ru)^2]. \tag{53}$$

Here $\kappa=A\beta\omega_0^2$, $d=c_0/\omega_0$, and $V(u'-ru)$ is of the form (3a) and (3b). By introducing

$$\zeta(u)=\exp[\tfrac{1}{2}\kappa d^2(1-r)u^2]h(u) \tag{54}$$

into (52) we can obtain a more symmetric form of the kernel, namely

$$\int \mathrm{d}u' \exp\{-\kappa[V(u'-ru)+\tfrac{1}{2}(1-r)^2\xi_s^2(u-u')^2]\}h(u')=\lambda h(u) \tag{55}$$

where we have accounted for (17) and (23a), ξ_s being the width of a static kink. Introducing the notation

$$K=Ac_0^2\beta \qquad \kappa=K\frac{\omega_0^2}{c_0^2}=K\theta \qquad \eta=\frac{1}{K(1+r)}=\frac{1}{\kappa(1-r)^2\xi_s^2} \tag{56}$$

equation (55) becomes

$$\sqrt{2\pi\eta}\int_{-\infty}^{+\infty}\mathrm{d}u' \exp[-\kappa V(u'-ru)]\exp\left(\frac{\eta}{2}\frac{\mathrm{d}^2}{\mathrm{d}u^2}\right)\delta(u-u')h(u')=\lambda h(u). \tag{55'}$$

Here by definition

$$\exp\left(-\frac{x^2}{2\eta}\right)=\sqrt{2\pi\eta}\exp\left(\frac{\eta}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\delta(x). \tag{57}$$

If both $\kappa\ll 1$ and $\eta\ll 1$, i.e. if

$$\theta\ll K^{-1}\ll 1 \tag{58}$$

then we can approximate the Baker-Hausdorff formula (Weiss and Maradudin 1962) by

$$\exp(\kappa A)\exp(\eta\beta) \simeq \exp(\eta\beta)\exp(\kappa A).$$

With this approximation the integration of (55′) yields

$$\left(-\frac{\eta}{2\kappa}\frac{d^2}{du^2}+V[(1-r)u]\right)h(u)=\varepsilon h(u) \tag{59}$$

where $\exp(-\kappa\varepsilon)=\lambda/\sqrt{2\pi\eta}$. Making a change of variable $x=(1-r)u$ and redefining the eigenfunction $h(x/(1-r))=\tilde{h}(x)$, equation (59) can be written as

$$\frac{d^2\tilde{h}}{dx^2}+2m^*(\varepsilon-V(x))\tilde{h}(x)=0 \tag{60}$$

with

$$m^*=\kappa^2\xi_s^2. \tag{61}$$

The form of (60) is exactly that encountered in the treatment of non-linear systems with NN interactions. However, the particulars of our long-range interaction problem are comprised of the large parameter m^*, the independent variable x and the redefined eigenfunction $\tilde{h}(x)$. By employing the generalised Langer transformation† (very adequate for problems with two turning points) (Nayfeh-Hasan 1973) used in a recent paper (Croitoru 1987), we succeed in determining the lowest eigenvalue of the isolated well in addition to the tunnel splitting of the degenerated isolated-well eigenvalue either into the lowest allowed band (SG) or into the two lowest allowed bands (DSG) due to the presence of the periodic sequence of the other wells. The compact expressions obtained for the eigenvalues corresponding to the bottom (b) and the top (t) of the lowest bands ($n=0, 1$) are listed below.

(i) SG system:

$$\varepsilon_b^{(0)} \simeq \varepsilon_{00}-t_0 \tag{62a}$$

$$\varepsilon_t^{(0)} \simeq \varepsilon_{00}+t_0 \tag{62b}$$

with

$$\varepsilon_{00} \simeq 1/2A\beta\omega_0^2\xi_s \tag{63}$$

being the lowest isolated-well eigenvalue and

$$t_0 \simeq [2^3/\sqrt{\pi}(m^*)^{1/4}]\exp(-\beta E_k) \tag{64}$$

being the tunneling rate where $E_k \simeq 8A\omega_0^2\xi_s$ approximates the energy of the static SG kink (with long-range interactions) and m^* is defined in (61). This approximation of the kink energy is justified since the parameter σ involved in (35a) is always small, allowing the series expansion of (35a).

(ii) DSG system

$$\varepsilon_b^{(0)} \simeq \varepsilon_{00}-(t_0^{(I)}+t_0^{(II)}) \tag{65a}$$

$$\varepsilon_t^{(0)} \simeq \varepsilon_{00}-(t_0^{(I)}-t_0^{(II)}) \tag{65b}$$

$$\varepsilon_b^{(1)} \simeq \varepsilon_{00}+(t_0^{(I)}-t_0^{(II)}) \tag{66a}$$

$$\varepsilon_t^{(1)} \simeq \varepsilon_{00}+(t_0^{(I)}+t_0^{(II)}) \tag{66b}$$

† For details concerning the application of the generalised Langer transformation to (60) with $V(\phi)$ defined in (3a) and (3b) the reader is referred to Croitoru (1987).

where $t_0^{(\mathrm{I,II})}$ are the tunneling rates through the type-I and type-II barriers, respectively and ε_{00} is the lowest isolated-well eigenvalue (63). The tunneling rates are

$$t_0^{(\mathrm{I,II})} \simeq \frac{1}{2}\frac{1}{\sqrt{\pi \mathrm{e}}}\frac{1}{\sqrt{m^*}} I^{(\mathrm{I,II})} \tag{67}$$

where

$$I^{(\mathrm{I})} = \exp\left(-2m^* \int_0^{\mu_1} \mathrm{d}x\sqrt{|q(x)|}\right)$$

$$\simeq 2^3\sqrt{\mathrm{e}}(m^*)^{1/4}\left(\sqrt{1-\alpha^2} - \frac{\alpha}{(1-\alpha^2)^{1/4}}\frac{1}{\sqrt{2}}\frac{1}{(m^*)^{1/8}}\right)\exp(-\beta E_k^{(\mathrm{I})}) \tag{68a}$$

$$I^{(\mathrm{II})} = \exp\left(-2m^* \int_{\mu_2}^{2\pi} \mathrm{d}x\sqrt{|q(x)|}\right)$$

$$\simeq 2^3\sqrt{\mathrm{e}}(m^*)^{1/4}\left(\sqrt{1-\alpha^2} + \frac{\alpha}{(1-\alpha^2)^{1/4}}\frac{1}{\sqrt{2}}\frac{1}{(m^*)^{1/8}}\right)\exp(-\beta E_k^{(\mathrm{II})}) \tag{68b}$$

with

$$E_k^{(\mathrm{I})} \simeq \frac{8A\omega_0^2\xi_s}{\sqrt{1-\alpha^2}}(\sqrt{1-\alpha^2} - \alpha\cos^{-1}\alpha) \tag{69a}$$

$$E_k^{(\mathrm{II})} \simeq \frac{8A\omega_0^2\xi_s}{\sqrt{1-\alpha^2}}(\sqrt{1-\alpha^2} + \alpha(\tfrac{1}{2}\pi + \cos^{-1}\alpha)). \tag{69b}$$

The superscripts (I, II) label the two different kink solutions. In the expressions (68*a*) and (68*b*), μ_1 and μ_2 represent the two turning points which result from $|q(x)| = |\varepsilon - V(x)| = 0$, and are approximately given by $\mu_1 \simeq \phi_1 - 2\sqrt{\frac{1}{2}\varepsilon}$, $\mu_2 \simeq \phi_1 + 2\sqrt{\frac{1}{2}\varepsilon}$, $V(x)$ being defined in (3*b*).

In the low-temperature regime the only contribution to the partition function stems from (62*a*) (SG system) and from (65*a*) (DSG system). Then the free energy per unit length will be

$$F = (1/\beta)\ln(\beta\hbar d\omega_0) + A\omega_0^2\varepsilon_{00} - A\omega_0^2 t_0 \tag{70}$$

where in the DSG case $t_0 = t_0^{(\mathrm{I})} + t_0^{(\mathrm{II})}$.

We remark that for both models, the kinks make major contributions to the free energy density, and consequently to all thermodynamic quantities which may be derived from it. For $\alpha = 0$, $t_0^{(\mathrm{I})} = t_0^{(\mathrm{II})}$ and we recover the SG result (64). We conclude this subsection with a final comment. For a given temperature β, the differential equation (60) will still include a large parameter $m^* = \kappa^2\xi_s$, if $\xi_s \to \infty$ ($r \to 1$). In this case, in accordance with (64), (67), (68*a*) and (68*b*), the tunnelling rates through the barriers will vanish, i.e. whatever the temperature may be we encounter an ordered phase. That certainly cannot be true; therefore the results obtained so far for small r cannot be extended to get information regarding the behaviour of the systems in the limit $r \to 1$. This limit has to be treated separately by another method (Sarker and Krumhansl 1981).

3.2. Van der Waals limit: $r \to 1$

Using (46*a*) together with (49*b*), the presence of the δ function allows us to write

$$\int_{-\infty}^{+\infty} \mathrm{d}\phi\, \exp(-\beta W(\phi) + K\phi x)g((1-r)\phi + rx) = \lambda g(x) \tag{71}$$

where we have made the change of variable

$$u = x/(1-r) \tag{72a}$$

and also redefined the eigenfunction $\zeta(u)$ as

$$\zeta(u) \Rightarrow g(x). \tag{72b}$$

The presence of the small parameter $1-r=\mu \ll 1$ enables us to approximate the eigenfunction $g(\mu\phi + rx)$ as follows:

$$g(x+\mu(\phi-x)) \simeq \exp[(\phi-x)q(x)]g(x) \tag{73}$$

where

$$q(x) = \mu g'(x)/g(x) \qquad g'(x) = \mathrm{d}g(x)/\mathrm{d}x. \tag{74}$$

Substituting (73) into (71) we obtain

$$\lambda = \int_{-\infty}^{+\infty} \mathrm{d}\phi \exp[-\beta W(\phi) + \phi(Kx + q(x))] \exp(-xq(x)). \tag{75}$$

The fact that the eigenvalue λ has to be independent of the variable x allows us to evaluate (75) for any value of x. The non-dependence of λ on x may also be expressed by setting $\mathrm{d}\lambda/\mathrm{d}x = 0$, a relation which leads to

$$q'(x) = \frac{KG(Kx+q(x)) - q(x)}{x - G(Kx+q(x))} \tag{76}$$

where, by definition,

$$G(\chi) = F'(\chi)/F(\chi) \tag{77}$$

with

$$F(\chi) = \int_{-\infty}^{+\infty} \mathrm{d}\phi \exp[-\beta W(\phi) + \phi\chi] \tag{78a}$$

$$F'(\chi) = \frac{\mathrm{d}F}{\mathrm{d}\chi} = \int_{-\infty}^{+\infty} \phi \, \mathrm{d}\phi \exp[-\beta W(\phi) + \phi\chi] \tag{78b}$$

and

$$\chi = Kx + q(x). \tag{79}$$

The existence of the expansion (73) requires that $q' = \mu(g''g - g'^2)/g^2$ has to be finite; therefore the denominator and numerator of (76) must vanish simultaneously. If they vanish at $x = x_0$ then the requirement stated above leads to the relations

$$Z_0 = Kx_0 + q(x_0) = 2KG(Z_0) \tag{80a}$$

and

$$q(x_0) = Kx_0. \tag{80b}$$

Then the eigenvalue λ_0 can be written

$$\lambda_0 = \exp(-Z_0^2/4K)F(Z_0) \tag{81}$$

and the free-energy density will be

$$F = -\frac{1}{2\beta}\ln\left(\frac{2\pi A}{\beta h}\right) - \frac{1}{\beta}\ln\lambda_0. \tag{82}$$

Knowing the formal expression for the free-energy density one can immediately deduce the internal energy, the specific heat and the magnetisation per particle (order parameter):

$$U = \tfrac{1}{2}k_B T - Z_0^2/4\beta K \tag{83}$$

$$\frac{1}{k_B} c_v = \frac{1}{2} + \frac{Z_0^2 G'(Z_0)}{1 - 2KG'(Z_0)} \qquad G' = \frac{dG}{dZ_0} \tag{84}$$

$$\langle \phi \rangle = m = \frac{\partial}{\partial(\beta H)} (-\beta F) = G(Z_0) = \frac{Z_0}{2K} \tag{85}$$

where H is the applied external field, and $G(Z_0) = G_0(Z_0 + \beta H)$ is defined by (77) with $W(\phi) = W_0(\phi) - H\phi$. The subscript zero refers to zero-field quantities. The relation (85) also holds for $H = 0$; then, if $Z = 0$, a spontaneous order will exist in the system. In the following we shall refer only to this latter situation. From the relations listed above it is evident that the basic quantity which has to be determined is Z_0; this can be achieved by resolving (80*a*) numerically. In the vicinity of the critical temperature this numerical evaluation of Z_0 can be avoided. Because of the fact that $G_0(Z_0)$ is an odd function of Z_0, (see equation (77)), $Z_0 = 0$ will be a solution of (80*a*). In the neighbourhood of this solution $G_0(Z_0)$ can be approximated by the series expansion

$$G_0(Z_0) \simeq b_0(K, \theta) Z_0 - b_1(K, \theta) Z_0^3 \ldots \tag{86}$$

where the subscript zero indicates the fact that we are looking for solutions in the absence of an external magnetic field. The parameter $\theta = \omega_0^2 / c_0^2$ defined in (56) varies from zero to infinity; in the following we shall investigate the behaviour of the systems under study in two limiting cases: (i) $\theta \to \infty$ (the coupling between the atoms is much weaker than the on-site potential) and (ii) $\theta \to 0$ (the coupling between the atoms is much stronger than the on-site potential). The coefficients b_0 and b_1 are positive quantities, and in general functions of K and θ. Taking into account (80*a*) and (86) we may write

$$Z_0^2 \simeq \frac{1}{2K} \frac{1}{b_1} (2Kb_0 - 1). \tag{87}$$

If $2Kb_0 < 1$ then the only solution of (80*a*) (the only real solution of (87)) will be $Z_0 = 0$. This regime corresponds to the disordered phase at high temperatures. If $2Kb_0 > 1$, then (87) also admits a non-zero real solution, and so does (80*a*). In this case an ordered phase exists. Consequently the critical temperature will result from

$$2K_c b_0(K_c, \theta) = 1. \tag{88}$$

Equation (87) tells us that the determination of Z_0 reduces to the evaluation of the two coefficients b_0 and b_1. The expressions for b_0 and b_1 are derived by Sarker and Krumhansl (1981) by expanding in power series of χ the functions $F(\chi)$ (78*a*), $F'(\chi)$ (78*b*) and $G(\chi)$ (77). The expressions they obtain are

$$b_0 = a_1 / a_0 \tag{89a}$$

$$b_1 = \tfrac{1}{6}(3b_0^2 - a_2/a_0) \tag{89b}$$

where

$$a_n = \int_{-\infty}^{+\infty} d\phi \, \phi^{2n} \exp[-K\theta V(\phi) - K\phi^2] \tag{90}$$

with $V(\phi)$ given by (3*a*) and (3*b*). The exponential factor $\exp(-K\phi^2)$, on the one hand, and the finite values taken by $V(\phi)$, on the other hand, ensure the convergence of the improper integral (90). Moreover, only minimal contributions to the integral (90) will be made by values of ϕ larger than those corresponding to the minima within a period. In contrast to the ϕ^4 system (Sarker and Krumhansl 1981), one cannot, in the SG and DSG models, establish a recurrence relation for the coefficients $\{a_n\}$. Consequently in order to evaluate b_1 (89*b*) one has to calculate a_2. Starting from the above relations (89*a*), (89*b*) and (90) and taking into account (3*a*) and (3*b*) as well as (84) we are in the position to determine the 'critical temperature' K_c^{-1} in the two stated limits. In the Ising limit $\theta \to \infty$, $b_0 = \pi^2$ (SG) and $b_0 = \phi_1^2$ (DSG), so the 'critical temperature' is $K_c^{-1} = 2\pi^2$ (SG) and $K_c^{-1} = 2\phi_1^2$ (DSG). In this limit, as expected, the magnetisation per particle (85) is given by

$$G_0(Z_0) = \pi \tanh(\pi Z_0) \qquad \text{SG case}$$

$$G_0(Z_0) = \phi_1 \tanh(\phi_1 Z_0) \qquad \text{DSG case}$$

being expressions characteristic of the Ising model.

As $\theta \to 0$ the integral (90) can be expanded about $\theta \to 0$, by performing integrals of the form

$$\int_{-\infty}^{+\infty} \mathrm{d}\phi\, \phi^{2n} \cos(a\phi) \cos(b\phi) \exp(-K\phi^2)$$

$$= \frac{\mathrm{d}^n}{\mathrm{d}K^n} \left\{ \frac{1}{2} \sqrt{\frac{\pi}{K}} \left[\exp\left(-\frac{(a-b)^2}{4K} \right) + \exp\left(-\frac{(a+b)^2}{4K} \right) \right] \right\} \tag{91}$$

(Gradshteyn and Ryzhik 1980) we obtain $K_c^{-1} = 4$ (SG) and $K_c^{-1} = 4(1-\alpha)/(1-\frac{1}{4}\alpha)$ (DSG), or for $\alpha \ll 1$, $K_c^{-1} \simeq 4(1-\frac{3}{4}\alpha-\frac{1}{4}\alpha^2)$. Finally, we shall make some comments regarding the behaviour in the critical region of both the magnetisation and the specific heat per particle. Expanding b_0 and b_1 about K_c, one finds that the magnetisation per particle diverges as

$$m = Z_0/2K \sim (T_c - T)^{1/2} \tag{92}$$

for both systems investigated in this paper.

Since for $T = T_c^+$ the only solution of (80*a*) is $Z_0 = 0$, the specific heat per particle (84) will be

$$c_v/k_B = \tfrac{1}{2} \qquad T = T_c^+ \tag{93a}$$

If $T = T_c^-$, (80*a*) also admits a solution $Z_0 \neq 0$ and the specific heat per particle becomes

$$\frac{c_v}{k_B} = \frac{1}{2} + \left[1 - \frac{2}{3} \frac{a_2(K_c, \theta)}{a_1(K_c, \theta)} \right]^{-1}$$

or

$$T = T_c^-. \tag{93b}$$

$$\frac{c_v}{k_B} = \frac{1}{2} + \frac{b_0^2(K_c, \theta)}{2b_1(K_c, \theta)}$$

In deriving these latter relations we made use of (84), (86), (88), (89*a*), (89*b*) and also (in the second expression) of (80*a*).

In the limit $\theta \to \infty$ we have

$$a_2(K_c)/a_1(K_c) \simeq \pi^2 \qquad K_c = 1/2\pi^2 \qquad \text{SG case}$$

and

$$a_2(K_c)/a_1(K_c) \simeq \phi_1^2 \qquad K_c = 1/2\phi_1^2 \qquad \text{DSG case.}$$

Then (93*b*) transforms into the known expression (Baker 1961, Sarker and Krumhansl 1981)

$$c_V/k_B = \tfrac{1}{2} + \tfrac{3}{2} \qquad T = T_c^- . \tag{93b'}$$

In the limit $\theta = 0$, both for the SG model and the DSG system, $a_2(K_c, 0)/a_1(K_c, 0) \simeq \frac{3}{2}(1/K_c)$, and consequently (93*b*) diverges for $\theta \to 0$, indicating another second-order phase transition. If we use the second expression of (93*b*) then the specific heat also diverges, due to the fact that $b_1 \simeq 0$ when $\theta = 0$. We note that if we apply (93*b*) to the ϕ^4 model, for the two limiting cases $\theta \to \infty$ and $\theta = 0$ we obtain the same behaviour as for the two models studied in the present paper. According to (93*b*), as long as $\theta \neq 0$ then the second-order phase transition is characterised by a finite jump in the specific heat per particle.

4. Conclusions

In the preceding sections we have presented the main features of two non-linear systems with long-range interactions of the Kac–Baker type. As we have pointed out, throughout this paper the formalism adopted for studying the SG and DSG models with long-range interactions has been that developed in Sarker and Krumhansl (1981) for the investigation of a ϕ^4 system with long-range interactions. The essential feature of this method is the conversion of all relevant expressions (equation of motion, potential energy, partition function) into equivalent expressions corresponding to problems with 'nearest-neighbour' interactions. In using this formalism we succeeded in deriving compact expressions for the kink solutions and kink energies. Whereas the kink solution and the kink energy for the SG model are represented by relatively simple closed-form expressions (27), (35*a*) and (35*b*), in the DSG case the two different kink solutions and their associated energies are given by rather complicated expressions (28*a*), (28*b*), (36*a*), (36*b*), (37*a*) and (37*b*), which also involve all three kinds of elliptical integrals. However, if the interaction-range parameter, r, is zero, these solutions reduce to the well known solutions either of the SG chain or the DSG model with NN interactions. From these relations it follows that as long as the parameter r assumes small values, for both systems studied here, the kinks are well defined 'elementary excitations' of finite width (static kink) and small activation energy. As the interaction range is increased ($r \to 1$) the kink width as well as the kink energy both become indefinitely large, i.e. the kink disappears. Although the kink solutions and kink energies differ from those of the ϕ^4 model, the qualitative behaviour is similar, as expected.

The thermodynamical properties of the SG and DSG models, have been investigated in two limiting cases: (i) small values of r and (ii) $r \to 1$ (van der Waals limit, infinite interaction range). Let us now summarise the characteristics of the thermodynamical behaviour of the two systems investigated in this paper in the limits stated above. For small values of r, we investigated the low-temperature thermodynamics of the SG and DSG systems by means of an asymptotic procedure adequate for solving the eigenvalue problem of a second-order differential equation which depends on a large parameter (Nayfeh-Hasan 1973, Croitoru 1987) and involves two turning points. In doing so we determined the temperature dependence of the free-energy density in the displacive limit. For both systems the free-energy density contains two parts: (i) a term which can be attributed to the free-energy density of a set of harmonic phonons when calculated to order $O(1/\xi_s)$ of the displacive limit; (ii) a term which can clearly be

associated with the kinks. In the SG case this latter term corresponds to the contribution of the single SG kink, while in the DSG case it involves the two DSG kinks. We remark, that this method also enabled us to determine the tunnel splitting of the lowest degenerate isolated-well eigenvalue into either one allowed narrow band (SG case) or into two allowed narrow bands (DSG case) for whose lower and upper extremities we obtained compact expressions (62)–(69). Furthermore we note that for a given temperature β the differential equation (60) still includes a large parameter if $\xi_s \to \infty$ ($r \to 1$). But in this case, in accordance with the expressions for the tunnelling rates (64), (67), (68*a*) and (68*b*), these latter will vanish due to the factor $\exp(-E_K\beta)$, E_K being the kink energy which in this limit becomes indefinitely large. This means that whatever the temperature may be, we encounter an ordered phase. As this cannot be true, the method adopted for small values of r does not allow us to extract conclusions about the behaviour of the systems as $r \to 1$. By using the procedure employed by Sarker and Krumhansl (1981) in this limit, we succeeded in demonstrating that for the infinite interaction range limit, the SG and DSG systems undergo a second-order phase transition. For the latter we determined the 'critical temperature' as well as the behaviour of the magnetisation and specific heat per particle in the critical region.

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