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Statistical mechanics of the continuum and discrete Φ^4 system with long-range interaction potential: the soliton dilute-gas phenomenology

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Abstract. The soliton dilute-gas phenomenology is used to study the statistical mechanics of the Φ^4 system with long-range interaction potential. Both the continuum and the discrete phonon excitations with their corresponding dispersion relations and non-linear excitations (walls or kinks) are investigated. In the continuum model, we show that the kink free energy and density decrease when the range of interaction increases. In the discrete model where the kink width is small, as a result of the collective coordinate method associated with Dirac's constrained Hamiltonian dynamics, the mass and the potential energy of kink vary periodically with the kink position in the lattice. This leads to a correction of the statistical results obtained in the continuum model.

1. Introduction

In the past few decades, a growing interest has been shown in the statistical mechanics of non-linear models of condensed-matter systems where the associated field equations of motion admit soliton solutions. In the continuum non-linear Klein–Gordon systems, such as Φ^4 and sine–Gordon models, which possess kink solutions (topological solitons), it has been shown, through the functional-integral technique or ideal-gas phenomenology, that the low-temperature thermodynamics of the systems are sensitive to and even dominated by solitons (Krumhansl and Schrieffer 1975, Mazenko and Sahni 1978, Schneider and Stoll 1980, Currie *et al* 1980). In particular, the presence of solitons in the system is signalled by a term proportional to $\exp(-E_k/k_B T)$ in the low-temperature free energy, where E_k is the energy of the soliton, k_B is the Boltzmann constant and T is the temperature.

The functional-integral technique has also been used to study the thermodynamics of the continuous system with long-range interaction of Kac–Baker type. By converting the functional integral into an equivalent nearest-neighbour problem, Sarker and Krumhansl (SK) (1981) evaluated the partition function of the long-range interaction model. They obtained the same proportional term and they concluded that, since E_k increases with increasing range of interactions while the proportional (exponential) term approaches zero, the long-range interaction system undergoes a second phase transition in the infinite-range limit.

All the aforementioned thermodynamics studies have been limited to the continuum models. The soliton (or the antisoliton) width has therefore been taken to be large enough to avoid the discreteness effects of the lattice. The soliton energy E_k was just a constant but, in some materials, the soliton extension is just a few lattice spacings (one or two) and the discreteness effects on soliton static and dynamical properties cannot be neglected (Woafo *et al* (1991) and references therein; hereafter, referred to as I).

In I, following initial investigations on the lattice discreteness, we have shown that in the long-range interaction system the kink energy varies periodically with the kink centre-of-mass position. The potential barrier and the pinning frequency suffered by the kink decrease when the range of interaction increases. Our purpose in this paper is to investigate the discreteness effects on the dilute-gas statistical mechanics of the long-range interaction Φ^4 systems. The influence of the range of interaction is considered. The organization of the paper is as follows.

In section 2, we present the discrete Φ^4 lattice with long-range interaction potential of Kac–Baker type. The various low-energy discrete excitations (phonons) of the resulting equation of motion are discussed with their corresponding dispersion relations. In the large-displacement regime, we show that the implicit kink solution of the continuum field can be adequately approximated by an explicit hyperbolic tangent profile (at least for some values of the range of interaction). The interaction between kinks and phonons is analysed through the linearized stability equation. Owing to the complexity of this equation whose explicit solution has not yet been obtained, an approximated phase shift which fits well with the short-range case is proposed.

In section 3, we review the results of the discreteness studies of I. In section 4, the ideal dilute-gas phenomenology calculations are presented. The grand partition function, the free energy and the density n of kinks and antikinks are evaluated both in the continuum and in the discrete limits. In the continuum limit, a comparison with the transfer-integral calculation performed by SK is made. In the discrete limit, it is seen that, owing to the X-dependence of the kink mass and kink energy (X is the position of the kink in the lattice), the discreteness causes corrections to the continuum statistical mechanics. These corrections are seen to disappear when the kink width increases. We show that the kink density decreases when the range of interaction increases. The temperature dependence of the kink density n is seen to appear through $\beta E_k^{(0)} = E_k^{(0)}/k_B T$ ($E_k^{(0)}$ is the rest energy of the kink).

Section 5 is devoted to a summary of our results.

2. The Φ^4 lattice with long-range interaction potential

The Hamiltonian of the discrete Φ^4 chain with long-range interaction potential has the form

$$H = \tfrac{1}{2}\sum_i \dot{y}_i^2 + \sum_i V(y_i) + \tfrac{1}{2}\sum_{j\neq i} V_{ij}(y_i - y_j)^2 \tag{1}$$

where y_i is a scalar dimensionless displacement of the ion i on a one-dimensional lattice. The equilibrium sites of ions are $x_i = ib$. The lattice spacing b is set equal to unity. The first term of the Hamiltonian (1) is the kinetic energy. The dot on y_i represents time differentiation. $V(y_i)$ is the double-well substrate potential with a pair of minima $y_i = \pm 1$. Its simplified form is

$$V(y_i) = \tfrac{1}{4}(y_i^2 - 1)^2. \tag{2}$$

The ions interact via a pair potential V_{ij} which is taken to be of Kac–Baker form (Baker 1961, Kac and Helfand 1973)

$$V_{ij} = [C(1-r)/2r]r^{|i-j|}. \tag{3}$$

C is a constant measuring the elastic energy of the lattice. r is the parameter which characterized the range of interaction with $0 \leqslant r < 1$. $|i-j|$ is the distance between ions on sites i and j. The virtue of this interaction potential, commonly encountered in physical systems such as an Ising ferromagnet lattice, is that the range of interaction can be varied continuously. The interaction between particles falls off exponentially as the separation between them increases. The pre-factor $1-r$ in equation (3) is chosen to ensure that the total potential experienced by one atom, due to all others, is finite in the thermodynamic limit where the number N of particles is infinite. This total potential is equal to $\sum_{j\neq i} V_{ij} = C$.

When $r = 0$, the model reduces to the well known Φ^4 chain with first-neighbour interactions. On the other hand, the limit $r \to 1$ which should be taken only when $N \to \infty$ defines the infinite-range problem. In the Hamiltonian (1), the potential energy of the discrete chain is the sum of the last two terms:

$$U = \tfrac{1}{2}\sum_{j\neq i} V_{ij}(y_i - y_j)^2 + \tfrac{1}{4}\sum_i (y_i^2 - 1)^2. \tag{4}$$

From the Hamiltonian (1), the equation of motion of the ith particle is

$$\ddot{y}_i - y_i + y_i^3 + [C(1-r)/r]\sum_{j\neq i} r^{|i-j|}(y_i - y_j) = 0. \tag{5}$$

Let

$$d = 1 - [C(1-r)/r]\sum_{j\neq i} r^{|i-j|} \doteq 1 - 2C \tag{6}$$

and define the auxiliary quantity (see SK)

$$L_i(y_i = [C(1-r)/r]\sum_{j\neq i} r^{|i-j|} y_j. \tag{7}$$

Equation (5) can be rewritten as

$$\ddot{y}_i - dy_i + y_i^3 = L_i(y_i). \tag{8}$$

$L_i(y_i)$ satisfies the recursive relation

$$(r + r^{-1})L_i = L_{i+1} + L_{i-1} + [C(1-r)/r](y_{i+1} + y_{i-1} - 2ry_i). \tag{9}$$

We can make the continuum approximation $y_i \to y(x,t)$, $L_i(t) \to L(x,t)$, to obtain the partial differential equation

$$r\ddot{y}_{xx} + [C(1+r) - r]y_{xx} + ry^3_{xx} - (1-r)^2(\ddot{y} + y^3 - y) = 0. \tag{10}$$

For $r = 0$, equation (10) reduces to the Φ^4 continuum equation (Krumhansl and Schrieffer 1975).

The discrete equation (8) and the continuum equation (10) have three trivial solutions which correspond to the unstable state $y_i = 0$ or $y = 0$ and the two stable states $y_i = \pm 1$. Apart from these solutions, there are other solutions of equation (8) and equation (10): the small-amplitude solutions which are discussed in section 2.1 and the soliton solution discussed in section 2.2. In section 2.3, we analyse the problem of interaction between the kink and phonons.

2.1. Discrete and continuum phonons

2.1.1. Case 1: oscillations about $y = 0$. The first small-amplitude states of the model are the unstable oscillations about the top of the double well ($y = 0$). Neglecting the non-linear term y_i^3 in equation (8) in view of finding linear wave solutions and using the recursive relation (9), one obtains the discrete equation

$$(r^2+1)\ddot{y}_i - r(\ddot{y}_{i+1}+\ddot{y}_{i-1}) = [r^2+1-2C(1+r)]y_i + [C(1+r)-r](y_{i+1}+y_{i-1}) \tag{11}$$

whose solution is

$$y_i = \alpha \sin(gi - \omega_g t)$$

with the discrete dispersion relation (α is the amplitude)

$$\omega_g^2 = \{r^2+1-2C(1+r)+2[C(1+r)-r]\cos g\}/[2r\cos g-(r^2+1)]. \tag{12a}$$

For small values of the dimensionless wavevector g, equation (12a) gives

$$\omega_g^2 = -1 + C(1+r)g^2/[(r-1)^2+rg^2] \tag{12b}$$

which is the continuum dispersion relation that can be obtained from the linear form of equation (10). In order that ω_g^2 (equation (12b)) be positive, g must satisfy the inequality relation

$$g^2 > (1-r)/[C(1+r)-r].$$

2.1.2. Case 2: oscillations about the bottom of the well $y_i = \pm 1$. This state corresponds to the situation in which all the particles are lowered to the bottom of one of the wells. Then we can write $y_i = \pm 1 + v_i$ where v_i is a linear wave. Substitution in equation (8) yields

$$(r^2+1)\ddot{v}_i - r(\ddot{v}_{i+1}+\ddot{v}_{i-1}) = -2[r^2+1+C(1+r)]v_i + [2r+C(1+r)](v_{i+1}+v_{i-1}). \tag{13}$$

Taking $v_i = \alpha\sin(gi - \omega_g t)$ and substituting in equation (13), we obtain the discrete dispersion relation

$$\omega_g^2 = \{-2[2r+C(1+r)]\cos g + [r^2+1+C(1+r)]\}/(r^2+1-2r\cos g). \tag{14a}$$

When $g \to 0$, equation (14a) reduces to

$$\omega_g^2 = 2 + C(1+r)g^2/[(r-1)^2+rg^2] \tag{14b}$$

which corresponds to the dispersion relation of the continuum model. It is obvious that, when $r = 0$, relations (14a) and (14b) reduce to the discrete and continuum dispersion relations of the Φ^4 chain with first-neighbour interactions. We shall refer to the dispersion relations (14a) and (14b) when studying the statistical mechanics of the system.

2.2. *Large-amplitude solutions*

For large-amplitude solutions (kinks), equation (8) is analytically intractable but, since its continuum form equation (10) can be solved, one can take its solution as the first-order solution of equation (8) (see I). Neglecting the fourth-order term $r\ddot{y}_{xx}$ in equation (10), in the spirit of the continuum approximation and because this term vanishes when $r \longrightarrow 0$ (or for zero-velocity solitons), the solution $y(x,t)$ of equation (10) is given by the implicit formula (SK)

$$\pm (x - Vt)/\sqrt{2}\xi = -3(\sigma/2)^{1/2}\sinh^{-1}[2\sigma/(1+\sigma)]^{1/2}y + (1+3\sigma)^{1/2}\tanh^{-1}\{[(1+3\sigma)/(1+\sigma+2\sigma^2 y)]^{1/2}y\} \tag{15}$$

where

$$\xi^2 = [C(1+r) - r - V^2(1-r)^2]/(1-r)^2 \tag{16a}$$

and

$$\sigma = r/(1-r)^2\xi^2. \tag{16b}$$

$y(x,t)$ is a topological soliton with a width measured by ξ and which propagates with a constant velocity V in the absence of perturbations. The positive (negative) sign corresponds to a kink (antikink).

In I, we have simplified the implicit solution (15) by the hyperbolic tangent waveform

$$y_k(x,t) = \pm\tanh[K(x - Vt)] \tag{17}$$

where

$$K^2 = 1/2\xi^2 = 1/2[C_0^2(r) - V^2] \tag{18a}$$

and

$$C_0^2(r) = [C(1+r) - r]/(1-r)^2 \tag{18b}$$

$K^{-1} = \sqrt{2}\xi$ defines the spatial extension of the kink. It increases indefinitely as the range of interaction tends to the infinite limit ($r \longrightarrow 1$).

There are two reasons which support the validity of the approximation (17). First, the soliton profile given by (15) suffers very slightly because of the approximation. Second, the soliton energy obtained in the continuum limit from (17) is

$$E_k = (2\sqrt{2}/3)\xi + (2\sqrt{2}/3)(V^2/\xi) \tag{19}$$

which approximately corresponds to

$$E_k = (2\sqrt{2}/3)\xi(1 + \tfrac{189}{640}\sigma - \tfrac{831}{8960}\sigma^2) + (2V^2/\xi\sqrt{2})(\tfrac{2}{3} + \tfrac{1}{15}\sigma - \tfrac{17}{252}\sigma^2)$$

calculated by SK from the implicit solution (15) (see the appendix where the integration of the kink energy is shown). However, one can note that the error between the two expressions increases with increasing range of interaction. For instance, for $r = 0.1$, the error is 2.9%; for $r = 0.4$, it is only 5.5% which is still acceptable. However, for $r = 0.5$, the error reaches 12.6% which already corresponds to a poor approximation.

Looking back at equation (19), one can easily show that the kink energy has the pseudo-relativistic form

$$E_{\mathrm{k}} = (E_{\mathrm{k}}^{(0)2} + P_{\mathrm{k}}^2 C_0^2)^{1/2} \tag{20}$$

where $P_{\mathrm{k}} = M_{\mathrm{k}} V(1 - V^2/C_0^2)^{-1/2}$ is the relativistic momentum and $E_{\mathrm{k}}^{(0)}$ is the rest energy of the kink (antikink):

$$E_{\mathrm{k}}^{(0)} = (2\sqrt{2}/3)C_0 = M_{\mathrm{k}} C_0^2 \tag{21}$$

where

$$M_{\mathrm{k}} = 2\sqrt{2}/3C_0 \tag{22}$$

is the kink rest mass. It is important to note that K^{-1} and E_{k} reduce, respectively, to the kink width and kink energy of the Φ^4 chain with nearest-neighbour interaction when $r = 0$. As the range of interaction increases (r increases), K^{-1} and E_{k} increase indefinitely. Consequently, such kinks become energetically less favourable for the system to support. They could no longer be considered in the low-temperature state.

2.3. Interaction between kink and phonons: an approximated phase shift calculation

The presence of kinks and phonons in the lattice produces a number of effects, characteristic of kink–kink and kink–phonon interactions. For instance, the continuum theory reveals that the phonon modes are distorted near the kink core. However, the important noticeable effect is that the occurrence of the interaction produces the phonon–kink and kink–phonon phase shifts. These shifts give complete information on the asymptotic behaviour of the linear and non-linear excitations after their collision in the lattice. Knowledge of the phase shifts is necessary when one wants to count the phonon states correctly in the presence of non-linear waves (Currie *et al* 1980, Theodorakopoulos 1982, Theodorakopoulos and Mertens 1983). In this work, we have assumed that there are no kink–kink (or kink–antikink) interactions. This is fulfilled when the separation between kinks and antikinks is at least equal to a kink thickness. We have also neglected the spatial shifts of the kinks due to their interactions with phonons.

In order to calculate the phonon phase shift due to the presence of soliton, one has to solve the linearized stability equation

$$r\ddot{Z}_{xx} - (1-r)^2\ddot{Z} + [C(1+r) - r + 3ry^2]Z_{xx} + 6r(y^2)_x Z_x + [3r(y^2)_{xx} - (1-r)^2(3y^2 - 1)]Z = 0 \tag{23}$$

obtained from (10) by substituting $y(x,t)$ by $y(x) + Z(x,t)$ with $Z \ll y$. Having regard to the asymptotic behaviour of equation (23), one obtains

$$r\ddot{Z}_{xx} + [C(1+r) + 2r]Z_{xx} - (1-r)^2(\ddot{Z} + 2Z) = 0. \tag{24}$$

Equation (24) corresponds to the continuum form of equation (13) which describes the oscillations of the particles near the bottom of the well. The resolution of equation (23) has appeared to be very difficult. To overcome the difficulty, we have made a crude assumption by converting the problem to one of finding the phase shifts in a simple Φ^4 chain which exhibits kinks or antikinks with profile given by (17). Therefore, we have obtained that the phonon phase shift can be approximated by (Wada and Schrieffer 1978)

$$\Delta(g) = 2\tan^{-1}[3Q/(Q^2-1)] \tag{25}$$

with $Q = \sqrt{2}gC_0(r)$. The r-dependence of $\Delta(g)$ is determined through $C_0(r)$. We note parenthetically that, when $r = 0$, $\Delta(g)$ reduces to the exact phonon phase shifts of the Φ^4 chain with nearest-neighbour interactions.

3. Discreteness effects in the long-range interaction chain

In I, we have used the collective coordinate method associated with Dirac's constrained Hamiltonian dynamics to study the motion of discrete kink in the Φ^4 chain with a long-range interaction potential. We have introduced new dynamical variables: the position $X(t)$ of the centre of the kink and the discrete fluctuations ψ_i on the continuum kink (17). The discrete kink therefore has the form

$$y_i = y_{\mathrm{k}}^i(X(t)) + \psi_i \tag{26}$$

where $y_{\mathrm{k}}^i(X(t)) = \tanh[K(i - X(t))]$ denotes the continuum kink at the discrete point i. $X(t)$, whose expression in the continuum limit is $Vt + X_0$ (where X_0 is the initial position of the soliton), is now promoted to the rank of any dynamical variable.

Decomposition (26) adds two more degrees of freedom to the system, corresponding to the collective coordinate $X(t)$ and its conjugate momentum P. Then it is followed by a set of two constraint conditions, for the coupling between the kink and the atomic degrees of freedom. The choice of the constraints is such that it decouples the degrees of freedom in the kinetic energy and minimizes ψ_i near the kink core. These constraints are

$$C_1 = \sum_i y_{\mathrm{k}}^{i(1)}\psi_i = 0 \qquad C_2 = \sum_i y_{\mathrm{k}}^{i(1)}\dot{\psi}_i = 0 \tag{27}$$

where $y_{\mathrm{k}}^{i(1)} = \mathrm{d}y_{\mathrm{k}}^i/\mathrm{d}X$. They have been shown to be second-class constraints in Dirac's terminology (Dirac 1964, Tomboulis 1975, Boesch and Willis 1990); since their Poisson brackets do not yield zero, this thus violates the requirements $C_1 = 0$ and $C_2 = 0$. Because of these constraints (in which the summation is replaced by integrals over the length of the lattice in the continuum limit), the formalism developed by Dirac for constrained dynamical systems has to be applied in order to derive the evolution equations of the variables X, ψ_i and their conjugate momenta. The correct equation of motion is therefore obtained through the Dirac brackets (Boesch and Willis 1990):

$$\{f,g\}^* = \{f,g\} + (1/M)(\{f,C_1\}\{C_2,g\} - \{f,C_2\}\{C_1,g\})$$

instead of the conventional Poisson brackets (without an asterisk). f and g are functions of the variables X, ψ_i and their momenta. M is defined below.

Using transformation (26) and constraints C_1 and C_2, the Hamiltonian (1) separates into three parts:

$$H = H_k + H_{ph} + H_{int} \tag{28a}$$

where

$$H_k = P^2/2M + U_0 + (E_1/2\pi)[1 - \cos(2\pi X)] \tag{28b}$$

is the kink effective Hamiltonian with (see I)

$$E_1 = [-r/6(1-r)^2]\{[C(1+r) - r]/rI_1 + J_1\}$$

where

$$I_1 = -8\pi^3 K^2 \sinh^{-1}(\pi^2/K)[2(q+1)/3 - 4(q+1)(q+4)/15]$$

$$J_1 = 24K^4\pi \sinh^{-1}(\pi^2/K)[-54(q+1)(q+4)(q+9)(q+16)/567$$
$$+788(q+1)(q+4)(q+9)/315 - 142(q+1)(q+4)/15 + 8(q+1)/3]$$

and

$$q = (\pi/K)^2.$$

$P = M\dot{X}$ is the kink momentum and M is the kink effective mass in the discrete lattice. It has the periodic structure

$$M = M_0 + M_1 \cos(2\pi X) \tag{28c}$$

with $M_0 = 4K/3$ and $M_1 = (8\pi^2/3)(q+1)\sinh^{-1}(\pi^2/K)$.

When the kink width increases, the kink potential energy reduces to the X-independent term U_0. The effect of the lattice discreteness is characterized by a shift in the rest energy of the kink. In the first-order approximation, this shift is obtained after a fourth-order expansion of the auxiliary quantity L_i while deriving the kink potential energy (see the appendix). U_0 is then given by the expression

$$U_0 = E_k^{(0)} - \tfrac{2}{15}[r/(1-r)^2]K^3\{[C(1+r) - r]/3r - \tfrac{1}{7}\}. \tag{28d}$$

The kink rest energy is therefore lowered below the continuum value $E_k^{(0)}$. Such lowering has also been obtained recently by other workers, in particular, by Trullinger and Sasaki (1987) while evaluating the first-order lattice discreteness corrections in the transfer-operator method for the kink-bearing systems and by Willis and Boesch (1990) when analysing a similar question (as ours) for the discrete sine–Gordon model.

The second term of the Hamiltonian (28a) is

$$H_{ph} = \tfrac{1}{2}\sum_i \dot{\psi}_i^2 + \sum_i \psi_i^2 + \tfrac{1}{2}\sum V_{ij}(\psi_i - \psi_j)^2 \tag{28e}$$

and consists of terms in ψ_i up to quadratic order. It is the Hamiltonian for phonons which oscillate about the bottom of the wells. The interaction between kinks and phonons is represented by

$$H_{int} = \sum[(y_k^i)^3 - y_k^i]\psi_i + \tfrac{3}{2} - \sum[(y_k^i)^2 - 1]\psi_i^2 + \sum V_{ij}(y_k^i - y_k^j)(\psi_i - \psi_j). \tag{28f}$$

As presented in section 2.3, this interaction Hamiltonian contributes to the phonon phase shifts.

4. Statistical mechanics: the ideal-gas phenomenology

In this section, we use the ideal-gas phenomenology developed by Currie *et al* (1980) to study the thermodynamic properties of the Φ^4 chain with long-range interactions. We consider first the state of low-energy excitations in which the particles oscillate about the bottom of the Φ^4 well. In this state, the excitations of the system are the classical harmonic phonons with dispersion relations given by (14*a*) and (14*b*). Therefore, the low-temperature free energy is given by

$$F_0 = (1/\beta)\int_0^{\pi} \mathrm{d}g\, \ln(\beta\hbar\omega_g) \tag{29a}$$

with $\hbar = h/2\pi$; h is the Planck constant. With the aid of a table of integrals (Gradshteyn and Ryzhik 1975), equation (29*a*) gives

$$F_0 = (\pi/\beta)\ln[\![\beta\hbar r^2 + 1 + C(1+r) + [(1-r)(1+r)^2 + 2C(1+r)]^{1/2}]\!] \tag{29b}$$

for the discrete model and

$$\begin{aligned} F_0 = (\pi/2\beta)(&\ln(\beta^2\hbar^2)\{2 + C(1+r)\pi^2/[r\pi^2 + (1-r)^2]\} + (2/\pi) \\ &\times\{2(1-r)^2/[2r+C(1+r)]\}^{1/2}\tan^{-1}\pi\{[2r+C(1+r)]/2(1-r)^2\}^{1/2} \\ &-(2/\pi)[(1-r)/\sqrt{r}]\tan^{-1}[\pi\sqrt{r}/(1-r)]) \end{aligned} \tag{29c}$$

for the continuum model. Equations (29*b*) and (29*c*) show a quantitative difference between the phonon contribution to the free-energy density in the discrete and the continuum limits. On the other hand, they show that the phonon contribution is always present for any range of interaction. As will be seen below, this is not the case for the soliton contribution.

When the system is in the large-amplitude regime, above the phonon excitations, kinks and antikinks (domain walls or simply walls) are generated. We are then in the presence of ensembles of phonons and walls. The presence of walls in the lattice induces a change in the phonon density of states and consequently leads to a thermal renormalization of the kink–phonon free energy. As previously emphasized by Currie *et al* (1980), correct counting of the phonon states in the presence of walls demands knowledge of the phonon phase shift (25). The change in the phonon density of states is then given by

$$\Delta\rho(g) = \rho(g) - \rho_0(g) = (1/2\pi)[\mathrm{d}\Delta(g)/\mathrm{d}g]. \tag{30}$$

$\rho_0(g) = L/2\pi$ is the unperturbed density of states and L is the length of the system considered to be large. $\rho(g)$ is the phonon density of states in the presence of domain walls. We have assumed that the phase shift in the discrete lattice is the same as in the continuum lattice although this assumption requires $g \ll 1$ (the continuum limit). See for instance the work by Theodorakopoulos *et al* (1980) where the properties of the discrete phase shift were determined.

Appealing to Levinson's theorem (Schift 1968) and to the Friedel (1952) sum rule, the total number of extended phonon states must be decreased by

$$P\int \mathrm{d}g\,\Delta\rho(g) = -N_b \tag{31}$$

where N_b is the number of bound states. P denotes the Cauchy principal value. The bound states and their frequencies are determined from the stability equation (23). Their accurate determination is not yet available since we have not succeeded in obtaining precise solutions of equation (23) but, in conformity with the approximation made in section 2.3, we can use the bound of the stability equation of kink (17) in the Φ^4 chain with nearest-neighbour interactions. Then, we have two bound states with frequences $\omega_{b1} = 0$ and $\omega_{b2} = 3$.

Considering walls moving at very low velocity, e.g. in the non-relativistic regime, the change in the phonon free energy due to the presence of walls is

$$\Delta F_0 = \frac{1}{\beta L} P \int_0^{\pi} \mathrm{d}g \, \ln(\beta \hbar \omega_g) \Delta \rho(g) \tag{32a}$$

which, with the aid of (30) and (31), can be rewritten as

$$\Delta F_0 = \frac{-N_b}{\beta L} \ln(\beta \hbar) + \frac{1}{2\pi\beta L} P \int_0^{\pi} \mathrm{d}g \, \mathrm{d}\Delta/\mathrm{d}g \, \ln(\omega_g). \tag{32b}$$

In view of the applicability of the phenomenological ideal-gas viewpoint, let us assume that in a low-temperature regime the phonons and domain walls are elementary distinguishable excitations. In addition, in order to neglect the interference of the walls, we assume that the separation between walls is at least equal to the wall thickness. The statistical problem of finding the characteristic contributions of phonons and walls to the equilibrium thermodynamic functions of our model is then that of a dilute gas of solitary waves and small-amplitude phonon excitations. The interactions between walls and phonons reside in the phase-shift function $\Delta(g)$ and is accommodated by the wall self-energy corrections defined as being equal to $L\Delta F_0$. In addition, the bound state with frequency ω_{b2} also contributes to the wall self-energy density by an amount $(1/\beta)\ln(\beta\hbar\omega_{b2})$. Then, the total wall self-energy is given by

$$\begin{aligned}\Sigma &= L\Delta F_0 + \frac{1}{\beta} - \ln(\beta\hbar\omega_{b2}) \\ &= \frac{-N_b}{\beta} \ln(\beta\hbar) + \frac{1}{\beta}\ln(\beta\hbar\omega_{b2}) + \frac{1}{2\beta\pi} P \int_0^{\pi} \mathrm{d}g \, \frac{\mathrm{d}\Delta}{\mathrm{d}g} \ln(\omega_g). \end{aligned} \tag{33}$$

In the course of calculating the contribution of the walls to the free energy of the system and finding the wall density, we have to consider the grand partition function (GPF). Considering that we have an ensemble of phonons, N_k kinks and $N_{\bar{k}}$ antikinks, we define the GPF by the relation (Currie *et al* 1980)

$$E = E^0 E_{k,\bar{k}} \tag{34}$$

where E^0 is the free GPF; $E^0 = \exp(-\beta L F_0)$ ($e \simeq 2.718$) with F_0 given by equation (29). $E_{k,\bar{k}}$ is the kink–antikink GPF defined in the Φ^4 model by

$$E_{k,\bar{k}} = \sum_{N=0} \exp(\beta\mu N) Z_{k,\bar{k}}(N) \tag{35}$$

where $Z_{k,\bar{k}}$ is defined in the discrete medium by

$$Z_{k,\bar{k}}^{di} = \frac{2}{N! h^N} \left(\int \exp\{-\beta[H_k(P,X) + \Sigma^{di}]\} \, \mathrm{d}X \, \mathrm{d}P \right)^N \tag{36a}$$

(since $U(X)$ is a periodic function) and in the continuum limit by

$$Z^{\mathrm{ci}}_{\mathrm{k},\bar{\mathrm{k}}} = \frac{2}{N!h^N}\left(\int_{-\infty}^{\infty} \exp[-\beta(E_{\mathrm{k}} + \Sigma^{\mathrm{ci}})]\,\mathrm{d}P_{\mathrm{k}}\right)^N . \tag{36b}$$

N is the total number of walls. That is $N = N_{\mathrm{k}} + N_{\bar{\mathrm{k}}} = 2N_{\mathrm{k}}$. We have assumed that there is no direct constraint applied toward kinks over antikinks. The winding number $N_{\mathrm{W}} = N_{\mathrm{k}} - N_{\bar{\mathrm{k}}}$ is then set equal to zero. The superscripts di and ci indicate respectively the discrete and the continuum index. μ is the wall chemical potential. The free-energy density (phonons + wall contributions) is

$$F = -(1/\beta L)\ln E = F_0 + F_{\mathrm{k},\bar{\mathrm{k}}} \tag{37}$$

where $F_{\mathrm{k},\bar{\mathrm{k}}}$ is the contribution of kinks and antikinks to the free-energy density. The average total wall number density $n = N/L$ is given by

$$n = -(\partial F/\partial\mu)_{T,L,\mu=0} \tag{38}$$

where one sets $\mu = 0$ after calculating the derivative of equation (37). μ is set equal to zero since there is no external constraint on the kink number.

The derivations are performed in section 4.1 for the continuum limit and in section 4.2 for the discrete limit.

4.1. Free energy and density of the walls in the continuum Φ^4 model with the long-range interaction potential

Inserting equation (20) into equation (36*b*) and restricting ourselves to the low-temperature regime, we obtain the expression for the kink–antikink GPF in the continuum chain as

$$E^{\mathrm{ci}}_{\mathrm{k},\bar{\mathrm{k}}} = \exp[(L/h)\alpha^{\mathrm{ci}}\exp(\beta\mu)] \tag{39}$$

where

$$\alpha^{\mathrm{ci}} = [E^{(0)}_{\mathrm{k}}/C_0(r)][2\pi/\beta E^{(0)}_{\mathrm{k}}]^{1/2}\exp[-\beta(E^{(0)}_{\mathrm{k}} + \Sigma^{\mathrm{ci}})]. \tag{40}$$

Considering (37) and (39), and after some rearrangement, one obtains

$$\begin{aligned} F^{\mathrm{ci}}_{\mathrm{k},\bar{\mathrm{k}}} &= -(1/\beta h)(4/\pi)(\pi^3/6\sqrt{2}\beta\xi)^{1/2}\exp(\beta\mu)\exp[-\beta(E^{(0)}_{\mathrm{k}} + \Sigma^{\mathrm{ci}})] \\ &= -\tfrac{1}{6}(4/\pi)(\pi/6\sqrt{2}\beta\xi)^{1/2}\exp(\sigma_{\mathrm{ci}})\exp(\beta\mu)\exp(-\beta E^{(0)}_{\mathrm{k}}) \end{aligned} \tag{41}$$

with

$$\sigma_{\mathrm{ci}} = -\frac{1}{2\pi}P\int_0^{\pi}\mathrm{d}g\,\frac{\mathrm{d}\Delta}{\mathrm{d}g}\ln(\omega^{\mathrm{ci}}_g). \tag{42}$$

Equation (41) gives the contribution of walls to the free energy in the continuum limit. It is seen that, when the range of interaction is small, the walls play an important role at low temperatures since $F_{\mathrm{k},\bar{\mathrm{k}}}$ is finite and different from zero. However, when the range of interaction increases, the wall contribution is found to vanish since $F_{\mathrm{k},\bar{\mathrm{k}}} \longrightarrow 0$.

Equation (41), with $\mu = 0$, should be compared with the contribution to the free-energy density of the walls given by

$$F^{\mathrm{ci}}_{\mathrm{k},\bar{\mathrm{k}}} = -(4/\pi)(e/\sqrt{2}\beta\xi)^{1/2}\exp(-\beta E^{(0)}_{\mathrm{k}})$$

obtained by the transfer-integral method (SK). Note that this last expression (given in our dimensionless parameters) does not include the factor $1/\beta$ which appears as an erroneous term in equation (73) of SK. Except for numerical pre-factors and the exponential term $\exp(\sigma_{\mathrm{ci}})$, the two expressions for $F^{\mathrm{ci}}_{\mathrm{k},\bar{\mathrm{k}}}$ give rise to the same qualitative results. We expect an improved transfer-integral method (Currie *et al* 1980) and more precise evaluation of σ_{ci} will lead to good agreement between the two results.

Differentiating equation (41) with respect to the chemical potential and setting $\mu = 0$ thereafter yield the low-temperature wall density in the continuum limit as

$$\begin{aligned} n^{\mathrm{ci}} &= (\beta/6\pi)(2\pi M_{\mathrm{k}}/\beta)^{1/2}\exp(\sigma_{\mathrm{ci}})\exp(-\beta E^{(0)}_{\mathrm{k}}) \\ &= (1/6\pi C_0)(2\pi)^{1/2}(\beta E^{(0)}_{\mathrm{k}})^{1/2}\exp(\sigma_{\mathrm{ci}})\exp(-\beta E^{(0)}_{\mathrm{k}}). \end{aligned} \tag{43}$$

This shows that the temperature dependence appearing in n^{ci} occurs through $\beta E^{(0)}_{\mathrm{k}} = E^{(0)}_{\mathrm{k}}/k_{\mathrm{B}}T$. One sees that n^{ci} decreases when r increases. This result is in accordance with the following predictions: since the kink width increases with increasing r, the number of non-interacting kinks must decrease. In the limit $r \longrightarrow 1$ (although less consistent here), $n^{\mathrm{ci}} \longrightarrow 0$. This confirms the fact that the system cannot support kinks and antikinks in the infinite-range limit.

4.2. Discreteness effects on the statistical properties of the model with the long-range interaction potential

In this section, we follow the order of calculation of section 4.1. A combination of equations (28) and (36*a*) yields

$$E^{\mathrm{di}}_{K,\bar{k}} = \exp[(1/h)\alpha^{\mathrm{di}}\exp(\beta\mu)] \tag{44}$$

with

$$\alpha^{\mathrm{di}} = \int \exp\{-\beta[H_{\mathrm{k}}(X,P) + \Sigma^{\mathrm{di}}]\}\,\mathrm{d}X\,\mathrm{d}P \tag{45a}$$

where $H_{\mathrm{k}}(X,P)$ is given by (28*b*). The phonon Hamiltonian contributes to F^{di}_0. The P-integration is just a Gaussian and yields $[2\pi M(X)/\beta]^{1/2}$.

The X-integration is over the entire length L of the system.

Then equation (45*a*) takes the form

$$\alpha^{\mathrm{di}} = \exp(-\beta\Sigma^{\mathrm{di}})\int_0^L \mathrm{d}X\,(2\pi M(X)/\beta)^{1/2}\exp[-\beta U_{\mathrm{k}}(X)] \tag{45b}$$

with

$$U_k(X) = U_0 + (E_1/2\pi)[1 - \cos(2\pi X)].$$

Substituting equations (44) and (45*b*) into (34) and using (37), one obtains the free energy of the wall in the discrete limit:

$$F^{\mathrm{di}}_{k,\bar{k}} = -\frac{1}{\beta L h}\exp(\beta\mu)\exp(-\beta\Sigma^{\mathrm{di}})\int_0^L \mathrm{d}X\left(\frac{2\pi M(X)}{\beta}\right)^{1/2}\exp[-\beta U_k(X)]. \tag{46}$$

Then the discrete kink and antikink density is

$$n^{\mathrm{di}} = \frac{\beta}{6\pi}\exp(\sigma_{\mathrm{di}})\frac{1}{L}\int_0^L \mathrm{d}X\left(\frac{2\pi M(X)}{\beta}\right)^{1/2}\exp[-\beta U_k(X)] \tag{47}$$

with

$$\sigma_{\mathrm{di}} = -\frac{1}{2\pi}P\int_0^\pi \mathrm{d}g\,\frac{\mathrm{d}\Delta}{\mathrm{d}g}\ln(\omega_g^{\mathrm{di}}).$$

If we make the assumption that $\sigma_{\mathrm{di}} \simeq \sigma_{\mathrm{ci}}$, then equation (47) can be rewritten as follows:

$$n^{\mathrm{di}} = n^{\mathrm{ci}}\frac{1}{L}\int_0^L \mathrm{d}X\left(\frac{M(X)}{M_k}\right)^{1/2}\exp\{-\beta[U_k(X) - E_k^{(0)}]\}. \tag{48}$$

This result, which has also been obtained by Willis and Boesch (1990) in the discrete sine–Gordon lattice, shows that the discreteness of the lattice is characterized by the X-integral, by the σ_{di} term and by the shift of the kink rest energy as it appears in equations (28*d*), (46) and (48). When the kink width increases, E_1 and M_1 tend to zero. Then $U_k \longrightarrow U_0$ and $M \longrightarrow M_0 = M_k$ since $K = 1/\sqrt{2}\xi$. This leads to a correction of the free energy and the wall density by an exponential term which depends on the rest energy shift $U_0 - E_k^{(0)}$ (Trullinger and Sasaki 1987, Willis and Boesch 1990). However, when the kink width is large enough, U_0 reduces to $E_k^{(0)}$ (since $K \longrightarrow 0$) and equations (46) and (48) reduce respectively to the continuum wall free-energy expression (41) and the continuum wall density (42).

5. Summary

In this paper, we have used the ideal-kink gas phenomenology to calculate the basic thermodynamic functions (free energy and density of walls) of the continuum and the discrete Φ^4 chain complicated with the long-range interaction potential of Kac–Baker type. Considering the non-relativistic and non-interacting walls, we have shown that the kink free energy and the kink density decrease when the range of interaction increases. This suggests that the kinks play a minimal role in determining the low-temperature properties of the system when the range of interaction is very long.

However, for the short-range interaction case, the kinks and antikinks play an important role in the low-energy excitations of the system, and contribute an exponential term $\exp(-\beta E_k^{(0)})$ to the free energy and to the density number.

When we take into account the lattice discreteness, the major effect is that the statistical results of the continuum model are corrected by an X-integral term and σ_{di}-term. These corrections, as expected, disappear when one approaches the continuum limit.

The basic results obtained in this paper can easily be used to determine other thermodynamic functions such as the internal energy density, the entropy and the specific heat of the long-range interactions model both in the continuum and in the discrete lattice. Another important point to outline is that, by setting $r = 0$, our results reduce to those obtained from the Φ^4 model with nearest-neighbour interactions.

In spite of the interesting results obtained in this paper, we mention that the problem of kink–phonon interaction in the model under consideration has been crudely approximated and requires a more precise analysis. For nearest-neighbour interaction models, a general kink density formula, which does not require explicit knowledge of the kink waveform or its small oscillations (e.g. the bound states and the phase shift), is known (DeLeonardis and Trullinger 1980). Investigations have been carried out with a view to applying this formula to the system with a long-range interaction potential.

Appendix

In this appendix, we present

(i) the expression for the kink energy in the continuum limit (see also SK) and
(ii) the appearance of the energy shift due to the lattice discreteness.

(i) The potential energy (4) can be written as

$$U = \sum_i \left(\tfrac{1}{4}(y_i^2 - 1)^2 + C y_i^2 - [C(1-r)/2r] \sum_j y_j r^{|i-j|} \right)$$
$$= \sum_i [\tfrac{1}{4}(y_i^2 - 1)^2 + C y_i^2 - \tfrac{1}{2} y_i L_i]. \tag{A1}$$

Using equation (8) and going to the continuum limit, we obtain

$$U = E_1 + E_2 \tag{A2}$$

where

$$E_1 = \tfrac{1}{4} \int_{-\infty}^{\infty} \mathrm{d}x \, (1 - y^4) \tag{A3}$$

and

$$E_2 = -\tfrac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}x \, y y_{tt}. \tag{A4}$$

Let $z = (x - Vt)/\xi$ and integrate by parts once. Then

$$E_2 = \frac{V^2}{2\xi}\int \mathrm{d}z\, y_z^2.$$

Substituting for y the kink implicit solution (15), one obtains with aid of a table of integrals

$$E_1 = (\xi/2\sqrt{\sigma})\{1 + (32\sigma)^{-1}(1+\sigma)(1-15\sigma)]\sinh^{-1}[2\sigma/(1+\sigma)]^{1/2} + (32\sigma)^{-1}[2\sigma(1+3\sigma)]^{1/2}(27\sigma - 1)\} \tag{A5}$$

and

$$E_2 = (V^2/\xi\sqrt{2})\{\tfrac{1}{9}[(1+3\sigma)/\sigma]^{3/2}\tan^{-1}\sqrt{\sigma} + [(1+9\sigma)/(18\sigma\sqrt{2\sigma})] \times \tanh^{-1}[2\sigma/(1+3\sigma)]^{1/2} - (6\sigma)^{-1}(1+3\sigma)^{1/2}\}. \tag{A6}$$

Since σ is a small parameter, we expand E_1 and E_2 in powers of σ. To order σ^2, this yields

$$E_1 = (2\sqrt{2}\xi/3)(1 + \tfrac{189}{640}\sigma - \tfrac{831}{8960}\sigma^2) \tag{A7}$$

and

$$E_2 = (V^2/\xi\sqrt{2})(\tfrac{2}{3} + \tfrac{1}{15}\sigma - \tfrac{17}{252}\sigma^2). \tag{A8}$$

When $r \longrightarrow 0$, E_1 and E_2 reduce to the first-order terms. If we recall that the kinetic energy is equal to E_2, the total kink energy is given by

$$E_\mathrm{k} = E_1 + 2E_2.$$

Note that, for small r, E_k reduces to equation (19) which is the kink energy with the explicit waveform (17). The kink rest energy in the continuum medium is

$$E_\mathrm{k}^{(0)} = E_1.$$

(ii) With a view to deriving the energy shift due to the lattice discreteness, we expand the recursive relation (9) up to the fourth-order term. Thus, one obtains, after replacing y_i by the first-order discrete solution f_i,

$$L_\mathrm{i} = -\mathrm{d}f_i + f_i^3 + (2/4!)[r/(1-r)^2]\{L_i^{(4i)} + [C(1-r)/r]f_i^{(4i)}\}. \tag{A9}$$

Inserting (A9) in (A1), using equation (8) and converting sums to integrals, we obtain for the zero-velocity kink

$$U_0 = E_\mathrm{k}^{(0)} - \tfrac{2}{15}[r/(1-r)^2]K^3[C(1+r)/3r - \tfrac{1}{7}]. \tag{A10}$$

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