Effect of solitons on the thermodynamic properties of a system with long-range interactions

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Thermodynamic properties of a one-dimensional "Φ^4" system, interacting via a pair potential which falls off exponentially with distance, is studied as a function of the range of this potential. From the classical equations of motion we find closed-form expressions for solitary wave solutions which reduce to Krumhansl and Schrieffer solutions in the short-range limit. The width and the energy (E_s) of the solitons are found to increase indefinitely as the range of the interaction increases. Transfer-integral techniques are used to evaluate the partition function by converting the functional integral into an equivalent nearest-neighbor problem. At low temperatures, the free energy contains a term proportional to $\exp(-E_s/k_BT)$ which signals the existence of solitons and ensures that there is no long-range order. However, when the range of interaction increases (i.e., E_s increases) this term approaches zero and the system undergoes a second-order phase transition in the infinite-range limit. The critical properties in this limit are found to be identical to a van der Waals model.

I. INTRODUCTION

It is well known[1] that a one-dimensional system with finite range interaction cannot exhibit a phase transition. The reason for this can be traced to the presence of low-lying excitations which destroy the long-range order in the system. An example is the one-dimensional Ising ferromagnet on a lattice in which spins which either can point up or down interact via a nearest-neighbor interaction of strength $-J$. In the ground state all the spins point either up or down, and are thus perfectly ordered, i.e., the magnetization is finite. The lowest excited states, however, are "kinks" or "domain walls" which consist of pairs of oppositely ordered sets of spins, and therefore have zero magnetization. The energy of a kink differs from the ground-state energy ($=-NJ$, where N is the number of spins) by an amount J. At low temperatures the thermal density of such kinks is then given by e^{-J/k_BT} which is nonzero as long as $T \neq 0$. Thus the magnetization or long-range order vanishes for any finite temperature.

Over the last few years a large number of physical systems have been identified in which various kinks, also known as solitary waves, or solitons, appear as natural low-lying excitations.[2] In most cases, these are localized large amplitude solutions of the governing equations and exhibit remarkable stability and other particlelike properties. Because of these properties, solitons have found wide spread use as models of extended particles in quantum field theories,[3] domain walls in ferromagnets[4] and ferroelectrics,[5] disgyration planes in superfluid ^{3}He,[6] and weakly pinned charge-density-wave condensates,[7] to mention a few.

Apart from their importance in the low-temperature thermodynamics, these solitons also play an important role in the dynamics of the system. A notable example is the so-called Φ^4 model which has been applied by Krumhansl and Schrieffer[5] (KS) to study the displacive phase transition in ferroelectrics. In addition to linear oscillations or phonons, KS find intrinsically nonlinear soliton solutions. By treating the solitons as a gas of weakly interacting particles they are able to calculate their contribution to the free energy at low temperature which agrees well with the results obtained from an exact calculation by a transfer integral method.[12] More importantly they can relate the central peak near $\omega = 0$ of the dynamic response function $S(q, \omega)$ with the motion of the solitons.

Recently, the ideas and methods of KS have been extended to other models exhibiting soliton excitations. These include, for example, the sine-Gordon chain[3,8,9] and a certain complex scalar field model.[10] In these systems the presence of the solitons is signaled by a term proportional to $\exp(-E_s/k_BT)$ in the low-temperature free energy, where E_s is the energy of the soliton.

Because of the mathematical complexity, most of the models studied to date have been limited to one dimension and to nearest-neighbor interactions only. Since such a system does not undergo a phase transition, it is not clear what roles, if any, solitons play in systems where there is a long-range order. One way to study this would be to consider two- or three-dimensional models; however, because of mathematical difficulties very few analytical results are known for dimensions greater than one, although computer simulations have been carried out in some cases.[11]

An alternative approach to the problem of phase transitions has been to introduce long-range interactions in one dimension. A well-studied example of such long-range interactions is the so-called Kac-Baker[14–16] potential in which the interaction between particles falls off exponentially as $e^{-\gamma x}$ as the separation x between them increases. This potential has been studied extensively in connection with the Ising[14–16] and the Potts's models,[17] mainly because analytic methods are available by which closed form expressions for various thermodynamic quantities can be obtained in the limit $\gamma \to 0$. These models are found to undergo a second-order phase transition as this limit is approached.

In this paper we study the "Φ^4" model with an exponential potential. In Sec. II we present the Hamiltonian and discuss the various low-energy solutions of the resulting equation of motion for the field. Closed-form expressions for the soliton solutions are obtained. As the range of the interaction increases both the width and the energy of the soliton are found to increase indefinitely with γ^{-1}. In Sec. III we use a transformation to convert the partition function into a functional integral in which the effective intreaction is nearest-neighbor type. Standard transfer integral technique[5,12] is then used to obtain the low-temperature properties for small γ^{-1}. The contribution of the solitons to the free energy is found to disappear as γ^{-1} increases. In Sec. IV the infinite range (van der Waals's) limit of the functional integral is discussed. As expected, the system is found to undergo a second-order phase transition. Various critical parameters are calculated, in particular the critical exponents are found to agree with those of the Ising model.[16] Conclusions and discussions are contained in Sec. V.

II. MODEL AND THE EXCITATIONS OF THE SYSTEM

We consider a system of ions (unit mass) placed on an infinite one-dimensional lattice of lattice spacing unity. The Hamiltonian is given by

$$H=\frac{1}{2}\sum_i \dot{u}_i^2+\sum_i \tilde{W}(u_i)+\frac{1}{2}\sum_{i\neq j} V_{ij}(u_i-u_j)^2 \quad . \tag{1}$$

Here i, j are the lattice points; u_i and $\dot{u}_i$ are the displacement and the velocity of the ith ion. The on-site potential $\tilde{W}(u_i)$ is the double-well type

$$\tilde{W}(u)=\frac{a}{4}(u^2-1)^2 \quad , \tag{2}$$

with a pair of minima at $u=\pm 1$. The ions are assumed to interact vía a pair potential V_{ij} which is taken to be of the Kac-Baker form

$$V_{ij}=\frac{J(1-r)}{2r}e^{-\gamma|i-j|} \quad , \tag{3}$$

where $r=e^{-\gamma}$ and J is a constant. γ^{-1} essentially defines the range of the interaction. The prefactor $(1-r)$ is chosen to ensure that the total potential experienced by one atom due to all others is finite for all r so that a thermodynamic limit exists.[13] With the above choice, this is obviously

$$\sum_{j\neq i} V_{ij}=\frac{J(1-r)}{2r}\sum_{j\neq i} r^{|j-i|}=J \quad ,$$

which is independent of the range of the interaction. Note also that because of the prefactor r^{-1}, the model reduces to a nearest-neighbor problem in the limit $r\to 0$, $\gamma\to\infty$. On the other hand, the limit $\gamma\to 0$, $r\to 1$ will define the infinite-range problem. For comparison we note that if in Ref. 5 we take $u_0=|A|/B=1$, $|A|=a$, $m=1$, $C=J$, and add a constant term $\frac{1}{4}$ for each lattice point then the KS Hamiltonian reduces to (1) in the limit $r\to 0$.

The equation of motion for u_i which follows from (1) is

$$\ddot{u}_i-a(u_i-u_i^3)+\frac{J(1-r)}{r}\sum_{j\neq i} r^{|j-i|}(u_i-u_j)=0 \quad . \tag{4}$$

Let

$$d=a-\frac{J(1-r)}{r}\sum_{j\neq i} r^{|j-i|}=a-2J \tag{5}$$

and

$$L_i=\ddot{u}_i-du_i+au_i^3 \quad . \tag{6}$$

Then Eq. (4) can be rewritten

$$L_i=\frac{J(1-r)}{r}\sum_{i\neq j} u_j r^{|j-i|} \quad . \tag{7}$$

Now,

$$L_{i+1}+L_{i-1}=\frac{J(1-r)}{r}\left[(r+r^{-1})\sum_{j\neq i} u_j r^{|j-i|}+(2ru_i-u_{i+1}-u_{i-1})\right] \quad . \tag{8}$$

From Eqs. (7) and (8) we obtain

$$(r+r^{-1})L_i=L_{i+1}+L_{i-1}+\frac{J(1-r)}{r}(u_{i+1}+u_{i-1}-2ru_i) \quad . \tag{9}$$

Notice that Eq. (9) contains only nearest-neighbor terms. It is precisely this property of the exponential interaction that enables one to obtain analytic results.

As in KS we now make the continuum approximation and write

$$u_i \to u(x), \quad L_i \to L(x) \ , \tag{10a}$$

$$u_{i+1} + u_{i-1} \simeq 2u(x) + \frac{\partial^2 u}{\partial x^2} \ , \tag{10b}$$

$$L_{i+1} + L_{i-1} \simeq 2L(x) + \frac{\partial^2 L}{\partial x^2} \ . \tag{10c}$$

Equation (9) then becomes

$$r u_{xxtt} + [J(1+r) - ar] u_{xx} + aru_{xx}^3 - (1-r)^2 (u_{tt} + au^3 - au) = 0 \ . \tag{11}$$

As expected, for $r=0$ this equation reduces to the KS form. Following KS we shall discuss the various solutions of Eq. (11).

A. Phonons

Case I: Oscillations about u = 0

This case corresponds to small amplitude oscillations about the top of the double well which is at a $a/4$ above the bottom of the wells. Neglecting the u^3 terms we obtain solutions of the form

$$u = \alpha \sin(qx - \omega t) \tag{12}$$

with the dispersion relation

$$\omega_q^2 = -a + \frac{J(1+r)q^2}{(r-1)^2 + rq^2} \ . \tag{13}$$

In order that ω_q^2 be positive q must satisfy

$$q^2 > (1-r)^2 a / [J(1+r) - ar] \ . \tag{14}$$

The energy of these phonons are given by

$$\epsilon_{\rm ph} = \tfrac{1}{4} La + \hbar\omega \ , \tag{15}$$

where the first term comes because each atom contributes $\frac{1}{4}a$ to the energy, with L as the length of the chain.

Case II: Oscillations about the bottom of the well

This case corresponds to the situation in which all the atoms are lowered to the bottom of one of the wells. We then write $u = \pm 1 + v$; to linear order v satisfies

$$r v_{xxtt} + [J(1+r) + 2ar] v_{xx} - (1-r)^2 (v_{tt} + 2av) = 0 \ . \tag{16}$$

The solutions are

$$u = \pm 1 + \alpha \sin(qx - \omega t) \tag{17a}$$

with the dispersion relation

$$\omega_q^2 = 2a + \frac{J(1+r)q^2}{(1-r)^2 + rq^2} \ . \tag{17b}$$

For these phonons there is a solution for any $q > 0$. We note that for a long chain, the energy of this state is much lower than the corresponding state in case I.

B. Solitons

To find the soliton solutions we turn our attention to the full nonlinear Eq. (11). The fourth-order term will be neglected in the spirit of the continuum approximation and also because this term vanishes for zero velocity solitons and/or for $r=0$. We look for solitons of the form $u = u(x - vt) = u(z)$, which gives

$$[J(1+r) - ar - v^2(1-r)^2] u_{zz} + aru_{zz}^3 - (1-r)^2 a (u^3 - u) = 0 \ . \tag{18}$$

Define

$$y = z/\xi \ , \tag{19a}$$

$$\xi^2 = \frac{J(1+r) - ar - v^2(1-r)^2}{a(1-r)^2} \ , \tag{19b}$$

$$\sigma = \frac{r}{(1-r)^2 \xi^2} \ . \tag{19c}$$

In terms of these variables Eq. (18) takes the form

$$\frac{d^2u}{dy^2} + u - u^3 + \sigma \frac{d^2}{dy^2} u^3 = 0 \ . \tag{20}$$

The solution which corresponds to a soliton can be obtained by imposing the boundary conditions $u \to \pm 1$, $du/dy \to 0$, as $y \to \pm\infty$. Then Eq. (20) can be integrated to give

$$\left[\frac{du}{dy}\right]^2 = \frac{(1-u^2)^2}{2(1+3\sigma u^2)^2} (2\sigma u^2 + 1 + \sigma) \ , \tag{21}$$

and

$$\pm \frac{y}{\sqrt{2}} = \int_0^u du \, \frac{1 + 3\sigma u^2}{(1-u^2)(1+\sigma+2\sigma u^2)^{1/2}} \tag{22}$$

$$= -3\left[\frac{\sigma}{2}\right]^{1/2} \sinh^{-1}\left[\frac{2\sigma}{1+\sigma}\right]^{1/2} u + (1+3\sigma)^{1/2} \tanh^{-1}\left[\left[\frac{1+3\sigma}{1+\sigma+2\sigma u^2}\right]^{1/2} u\right] \ . \tag{23}$$

As $r \to 0$, $\sigma \to 0$ and Eq. (23) reduces to the KS

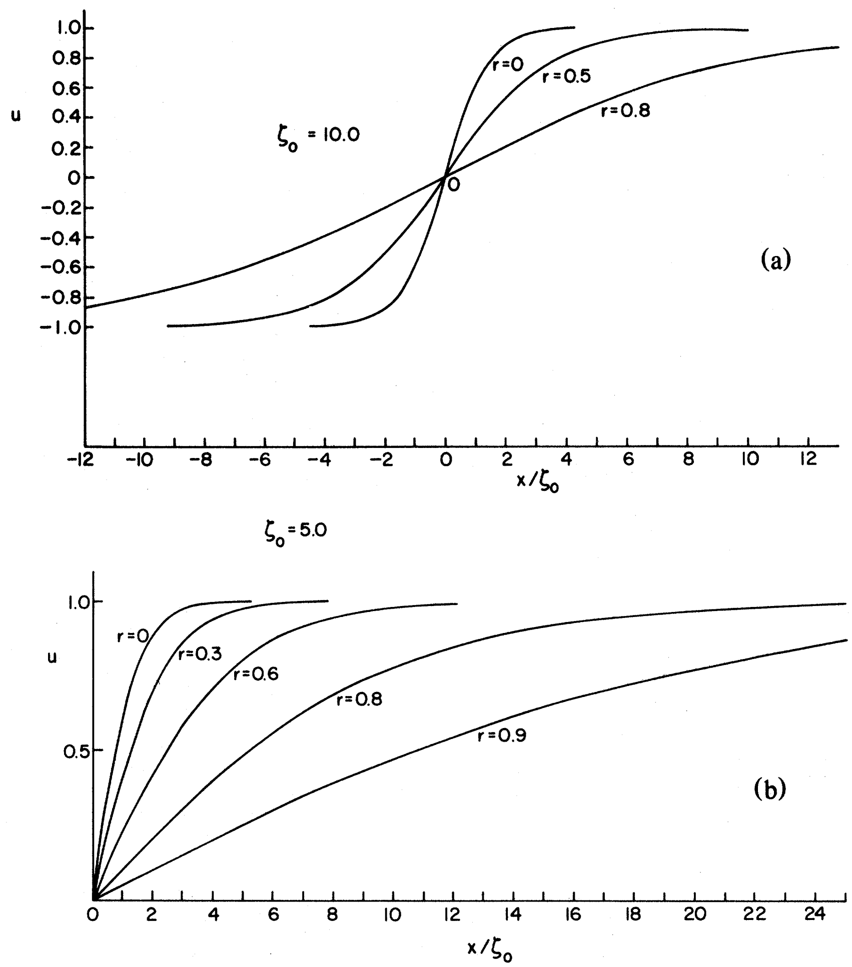

FIG. 1. Soliton profiles for (a) $\zeta_0 = J/a = 10$ and (b) $\zeta_0 = 5$ for various values of the range parameter $r = e^{-\gamma}$. Note the increase in the width of the soliton as the range increases.

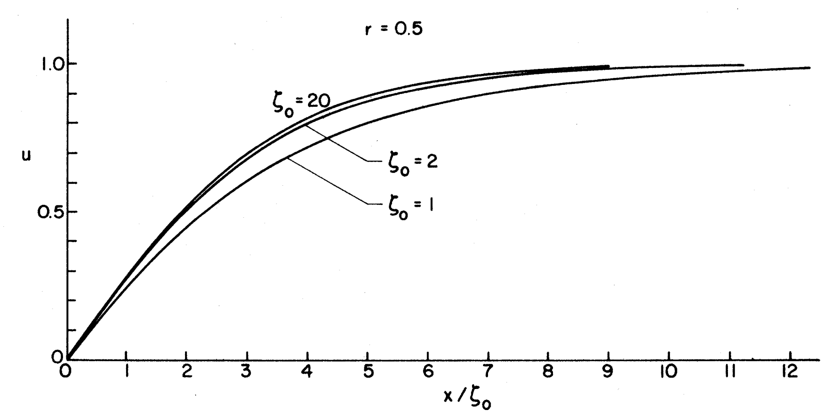

FIG. 2. Soliton profiles for $r = 0.5$ and for various values of $\zeta_0 = J/a$.

form

$$u = \pm \tanh y/\sqrt{2} \ , \tag{24}$$

where the positive (negative) sign corresponds to a soliton (antisoliton).

The parameter ξ has the dimensions of length and gives a measure of the width of the soliton. As $r \to 0$, ξ reduces to $\xi_{KS} = [(J - v^2)/a]^{1/2}$. Since ξ should be greater than a lattice spacing we require that $J > a$. In the limit $r \to 1$, ξ diverges as $(1-r)^{-1}$. However, the parameter σ remains small throughout and approaches $a/(2J-a)$ as $r \to 1$. We note the σ-dependent term breaks the Lorentz invariance of the short-range problem. Since ξ diverges as $(1-r)^{-1}$, the kink slowly disappears as $r \to 1$. This is shown in Fig. 1 where u is plotted against x/ζ_0 for $v=0$ solitons, with $\zeta_0 = \xi_{KS}(v=0) = J/A$. In the limit $r \to 1$, the width of the soliton becomes infinite and $u \to 0$ for all x. This corresponds to the case in which all the particles sit at the top of the well and has a high energy as is shown below. We have also plotted u vs x/ζ_0 for different values of ζ_0 and for $r = 0.5$ (Fig. 2). We see that the shape of the curve changes very little as the ζ_0 is measured from 2 to 20.

C. Energy of the soliton

The potential energy can be written

$$E_p = \sum_i \left[\frac{a}{4}(u_i^2 - 1)^2 + J u_i^2 - \frac{J(1-r)u_i}{2r} \sum_{j \neq i} u_j r^{|j-i|} \right]$$

$$= \sum_i \left[\frac{a}{4}(u_i^2-1)^2 + J u_i^2 - \tfrac{1}{2} u_i L_i \right] \ , \tag{25}$$

where we have used the equation of motion (7). Using (6) and going to the continuum limit we obtain

$$E_p = E_1 + E_2 \ , \tag{26}$$

where

$$E_1 = \frac{a}{4} \int_{-\infty}^{\infty} dx\, (1 - u^4) \tag{27}$$

and

$$E_2 = -\tfrac{1}{2} \int_{-\infty}^{\infty} dx\, u u_{tt} \ . \tag{28}$$

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

$$E_2 = \frac{v^2}{2\xi} \int_{-\infty}^{\infty} dy\, u_y^2 \ . \tag{29}$$

Also

$$E_k = \frac{v^2}{2\xi} \int_{-\infty}^{\infty} dx\, u_t^2 = \frac{v^2}{2\xi} \int_{-\infty}^{\infty} dy\, u_y^2 = E_2 \ , \tag{30}$$

where E_k is the kinetic energy. Substituting for u the soliton solution (23) we obtain after considerable algebra

$$E_1 = \frac{a\xi}{2\sqrt{\sigma}} \left[\left(1 + \frac{1}{32\sigma}(1+\sigma)(1-15\sigma) \right) \sinh^{-1}\left(\frac{2\sigma}{1+\sigma} \right)^{1/2} + \frac{1}{32\sigma}[2\sigma(1+3\sigma)]^{1/2}(27\sigma - 1) \right] \tag{31}$$

and

$$E_2 = \frac{v^2}{\xi\sqrt{2}} \left[\frac{1}{9} \left(\frac{1+3\sigma}{\sigma} \right)^{3/2} \tan^{-1}\sqrt{\sigma} + \frac{1+9\sigma}{18\sigma\sqrt{2\sigma}} \tanh^{-1}\left(\frac{2\sigma}{1+3\sigma} \right)^{1/2} - \frac{1}{6\sigma}(1+3\sigma)^{1/2} \right] \ . \tag{32}$$

Since $\sigma \to 0$ as $r \to 0$, and σ remains a small parameter even when $r \to 1$, we can expand Eqs. (31) and (32) in powers of σ. To order σ^2 this yields

$$E_1 = \frac{2\sqrt{2}a\xi}{3}\left(1 + \tfrac{189}{640}\sigma - \tfrac{831}{8960}\sigma^2\right) \tag{33}$$

and

$$E_2 = \frac{v^2}{\xi\sqrt{2}}\left(\tfrac{2}{3} + \tfrac{1}{15}\sigma - \tfrac{17}{252}\sigma^2\right) \ . \tag{34}$$

Note that in the limit $r \to 0$ Eqs. (33) and (34) reduce to the short-range values. Equations (31) and (32) are very well approximated by (34) and (35) for all σ. Even when $\sigma = \sigma_{max} = 1$, the error is only about 6%. Since $E_1 \propto \xi$, the energy of the soliton increases indefinitely as $r \to 1$. These solitons therefore play a minimal role in determining the low-temperature properties of the system when the range of the interaction is very long. In particular, they can not destroy the order of the low-temperature phase in the van der Waals's limit. However, for small r they constitute important low-energy excitation of the system, and contribute an exponential term to the free energy as we shall see in Sec. III.

III. STATISTICAL MECHANICS

The thermodynamic quantities are derived from the partition function which can be written as a functional integral over the field variables u_i and $p_i = \dot{u}_i$

$$Z = \int \prod_{i=1}^{N} du_i \prod_{i=1}^{N} dp_i \exp[-\beta H(\{p_i, u_i\})] \ , \tag{35}$$

where $\beta = 1/k_B T$ and N is the number of atoms.

For classical fields the integrations over u and p factorize and we have

$$Z = Z_p Z_u \quad (36)$$

with

$$Z_p = \int_{-\infty}^{\infty} \cdots \int \left[\prod_{i=1}^{N} dp_i\right] \exp\left[-\beta \sum_{i=1}^{N} \frac{p_i^2}{2m}\right] = \left[\frac{2\pi}{\beta}\right]^N , \quad m = 1 \quad (37)$$

and

$$Z_u = \int_{-\infty}^{\infty} \cdots \int \left[\prod_{i=1}^{N} du_i\right] \exp[-\beta V(\{u_i\})] , \quad (38)$$

where

$$V(u_i) = \sum_i \frac{a}{4}(u_i^2 - 1)^2 + \frac{J(1-r)}{4r} \sum_{i \neq j} (u_i - u_j)^2 r^{|i-j|} . \quad (39)$$

In general the evaluation of Z_u in closed form is very difficult, if not impossible. For nearest-neighbor interactions the problem can be transformed into one of finding the largest eigenvalue of a transfer-integral equation. In one dimension one can solve this equation at least numerically and thereby calculate all the thermodynamic quantities of interest. KS[5] have used this technique based on a method of Scalapino, Sears, and Ferrell[12] to study the low-temperature behavior of the short-range ($r = 0$) problem. For long-range interactions, however, the reduction of the problem to one of solving an integral equation is, in general, not possible. The Kac-Baker potential proves to be an exception to this rule in that the functional integral for Z_u can be transformed into an equivalent nearest-neighbor problem. We now show how this reduction can be achieved.

A. Integral equation

We start by rewriting Z_u as

$$Z_u = \int_{-\infty}^{\infty} \cdots \int \left[\prod_i du_i \, e^{-\beta W(u_i)}\right] \exp\left[\frac{K(1-r)}{r} \sum_{j>i} u_i u_j r^{|j-i|}\right] , \quad (40)$$

where $W(u)$ is the on-site potential

$$W(u) = \tfrac{1}{4} a (u^2 - 1)^2 + J u^2 \quad (41)$$

and $K = \beta J$.

One can, in principle, also include a term linear in u which describes the coupling of the displacement field u to an externally applied field. The following analysis is valid for any form of the local potential $W(u)$. Kac and Helfand[14,15] have shown that Eq. (40) can be converted into a nearest-neighbor problem and therefore can be written in terms of an integral operator which repeatedly operates on a complete set of functions. Although their integral equation is well suited for analysis near the van der Waals limit ($r = 1$), for arbitrary r it is not easy to analyze and in particular, it does not reduce to the integral equation of KS in the limit $r \to 0$. Baker,[16] on the other hand, used an ingeneous transformation to derive a different integral equation which reduces to the corresponding short-range transfer integral. His analysis, however, is only valid for the Ising model ($u = \pm 1$) in zero magnetic field. In what follows we show that a Baker-type equation, which reduces to the KS form in the limit $r \to 0$, can be obtained for general type of field variables u and for arbitrary local interaction $W(u)$.

To derive this equation we first define the auxiliary field variable y_i by

$$y_i = \sum_{j=i}^{N} r^{j-i} u_j . \quad (42)$$

Then the y's satisfy the recursion relations

$$y_j = u_j + r y_{j+1}, \quad j = 1, 2, \ldots, N-1 \quad (43a)$$

$$y_N = u_N . \quad (43b)$$

Using (43) the interaction term can be rewritten

$$\frac{K(1-r)}{r} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} u_i u_j r^{j-i} = K(1-r) \sum_{i=1}^{N-1} u_i y_{i+1} . \quad (44)$$

The partition function then becomes

$$Z_u = \int_{-\infty}^{\infty} \int \left[\prod_i du_i \, dy_i\right] \exp\left[-\beta \sum_{i=1}^{N} W(u_i) + K(1-r) \sum_{i=1}^{N-1} u_i y_{i+1}\right] \left[\prod_{i=1}^{N-1} \delta(y_i - u_i - r y_{i+1})\right] \delta(y_N - u_N) . \quad (45)$$

The δ functions ensure that the integrations over the auxiliary variables y_i are restricted by Eq. (43). Note that the original field variables u_i are now decoupled and therefore can be integrated out. Define

$$G(y,y')=\int_{-\infty}^{\infty}du\,\exp[-\beta W(u)+K(1-r)uy']\delta(y-u-ry') \quad (46a)$$

$$=\exp[-\beta W(y-ry')+K(1-r)y'(y-ry)]\ , \quad (46b)$$

and

$$F(y)=\int_{-\infty}^{\infty}du\, e^{-\beta W(u)}\delta(y-u)=e^{-\beta W(y)}\ , \quad (47)$$

so that the partition function takes the form

$$Z_u=\int_{-\infty}^{\infty}\int\prod_{i=1}^{N}dy_i\left[\prod_{i=1}^{N-1}G(y_i,y_{i+1})\right]F(y_N)\ . \quad (48)$$

We have thus arrived at a nearest-neighbor problem. Equation (48) is valid for any type of field variable (discrete or continuous) and any form of the local interaction $W(u)$.

Since $G(y,y')$ couples only nearest neighbors the integral in Eq. (48) can be regarded as a repeated operation of an integral operator. As it stands, $G(y,y')$ is not symmetric in y and y', therefore we express the kernel G in terms of left and right eigenvectors

$$G(y,y')=\sum_m \lambda_m\,\Psi_m(y)\Phi_m(y') \quad (49)$$

with the normalization

$$\int_{-\infty}^{\infty}dy\,\Psi_m(y)\Phi_n(y)=\delta_{mn}\ . \quad (50)$$

Putting (49) in (48) and using (50) one obtains

$$Z_u=\sum_m A_m B_m \lambda_m^{N-1}\ , \quad (51)$$

where

$$A_m=\int_{-\infty}^{\infty}dy\,\Psi_m(y) \quad (52a)$$

and

$$B_m=\int_{-\infty}^{\infty}dy\,e^{-\beta W(y)}\Phi_m(y)\ . \quad (52b)$$

The eigenvalues are given by

$$\lambda_m\Psi_m(y)=\int_{-\infty}^{\infty}dy'\,G(y,y')\Psi_m(y')\ , \quad (53)$$

$$\lambda_m\Phi_m(y)=\int_{-\infty}^{\infty}dy'\,G(y',y)\Phi_m(y')\ . \quad (54)$$

To obtain the eigenvalues we need to solve only one of these equations.

We note that if $W(y)=W(-y)$, then the kernel G has definite parity, i.e., $G(y,y')=G(-y,-y')$. The functions $\Phi(y)$ and $\Psi(y)$ are then either even or odd. For even functions (54) reduces to Baker's functional equation for the Ising model. This equation has also been derived by Viswanathan and Meyer[17] in connection with the Ising and Potts's models by a different method. They have shown that the eigenvalues are real and the largest eigenvalue is positive.

Since the analysis is valid for arbitrary number of atoms, the quantities A_m,B_m must be finite, for otherwise the partition function will be infinite for a finite chain. The free energy per particle is then given by

$$\frac{\beta F}{N}=-\frac{1}{N}\ln Z=-\frac{1}{2}\ln\left[\frac{2\pi}{\beta}\right]-\frac{1}{N}\ln Z_u\ . \quad (55)$$

In the thermodynamic limit this gives

$$\lim_{N\to\infty}\frac{\beta F}{N}=-\frac{1}{2}\ln\left[\frac{2\pi}{\beta}\right]-\ln\lambda_0\ , \quad (56)$$

where λ_0 is the largest eigenvalue of Eqs. (53) and (54). Various thermodynamic quantities can be extracted from Eq. (56) by standard means.

B. Low temperature properties near $r=0$

We have already noted in Sec. II that near $r=0$ the solitons can be regarded as low-energy excitations and therefore should show up in the free energy at low temperatures. When r is exactly equal to zero Eq. (54) reduces to

$$\lambda\Phi(y)=\int_{-\infty}^{\infty}dy\,\exp[-\beta W(y')+Kyy']\Phi(y')\ . \quad (57)$$

Let

$$\Phi(y)=\exp\left[\frac{\beta a}{4}(y^4-2y^2)+Ky^2\right]h(y)\ . \quad (58)$$

Then $h(y)$ satisfies

$$\lambda h(y)=\exp\left[-\frac{\alpha}{4}(y^2-1)^2\right]\times\int_{-\infty}^{\infty}dy'\exp\left[-\frac{K}{2}(y-y')^2\right]h(y')\ , \quad (59)$$

where $\alpha=\beta a=K\theta$, with $\theta=a/J$.

This is precisely the KS integral equation for the short-range problem.[5] Following the method of Scalapino, Sears, and Ferrell,[12] KS have converted this equation into an effective Schrödinger equation, valid in the "displacive regime" (small θ). We shall use the same technique to extract the low-temperature behavior of our model for small but nonzero r. The simplicity in (59) arises because the integrand depends only on the differences $y-y'$. Since for finite r the kernel is not symmetric in y and y', such a simplification is not possible. To make the kernel as symmetric as possible, let us define

$$\Phi(y)=\exp\left[\frac{\alpha}{8}(1-r)^2(1-r^2)y^4-\tfrac{1}{4}(\alpha-2K)(1-r^2)y^2\right]h(y) \quad . \tag{60}$$

Then $h(y)$ satisfies

$$\lambda h(y)=e^{-\alpha/4}\int_{-\infty}^{\infty}dy'\exp\left[\frac{\alpha}{8}(1-r^2)(1-r)^2(y'^4-y^4)-y^4)-\frac{\alpha}{4}(y'-ry)^4\right]$$
$$\times\exp\left[\frac{\alpha}{4}(1-r)^2(y^2+y'^2)-\tfrac{1}{2}[K(1+r)-\alpha r](y-y')^2\right]h(y') \quad . \tag{61}$$

In (61) only the quartic term in the exponential is not symmetric in y and y'. However, for $r=0$ and 1, the kernel is symmetric. For small r an effective Schrödinger equation can be obtained as follows. First, consider the identity

$$e^{-x^2/2\eta}=\sqrt{2\pi\eta}\,\exp\left[\frac{\eta}{2}\frac{d^2}{dx^2}\right]\delta(x) \quad , \tag{62}$$

which can be easily established by using the definition of the δ function

$$\delta(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dq\,e^{iqx} \quad . \tag{63}$$

Using (62) in (61) with $\eta=[K(1+r)-\alpha r]^{-1}$ we obtain

$$\lambda h(y)=(2\pi\eta)^{1/2}e^{-\alpha/4}\int_{-\infty}^{\infty}dy'\exp\left[\frac{\alpha}{8}(1-r)^2(1-r^2)(y'^4-y^4)-\frac{\alpha}{4}(y'-ry)^4+\frac{\alpha}{4}(1-r)^2(y^2+y'^2)\right]$$
$$\times\exp\left[\frac{\eta}{2}\frac{\partial^2}{\partial y^2}\right]\delta(y-y')h(y') \quad . \tag{64}$$

At this point complication arises because of the noncommutativity of the operator $\partial^2/\partial y^2$ with the rest of integrand. However, if both α and η are small then we can use the well-known Baker-Hardsdorff[18] formula

$$e^{\alpha A}e^{\eta B}\simeq e^{\alpha A+\eta B}\simeq e^{\eta B}e^{\alpha A} \quad . \tag{65}$$

Corrections involving commutators of A and B are higher orders in η and α. Since $\eta\propto K^{-1}$ and $\alpha=K(a/J)=K\theta$ these parameters will be small only if $\theta\ll K^{-1}\ll 1$. However, the work of Guyer and Miller[19] on the sine-Gordon system indicates that even if $K\theta>1$, Eqs. (64) and (67) would yield the same result for the largest eigenvalue as long as $\theta\ll 1$ and $K^{-1}\ll 1$. Using (65) the operator $\exp(\frac{1}{2}\eta\partial^2)/\partial y^2$ can be taken outside the integral (64) and the integration over the variable y' then yields

$$\lambda h(y)\simeq(2\pi\eta)^{1/2}\exp\left[-\frac{\alpha}{4}+\frac{\eta}{2}\frac{d^2}{dy^2}\right]\exp\left[-\frac{\alpha}{4}(1-r)^4y^4+\frac{\alpha}{2}(1-r)^2y^2\right]h(y)$$
$$\simeq(2\pi\eta)^{1/2}\exp\left[\frac{\eta}{2}\frac{d^2}{dy^2}-\frac{\alpha}{4}[(1-r)^2y^2-1]^2\right]h(y) \quad , \tag{66}$$

where we have again used (65). Defining $\lambda=(2\pi\eta)^{1/2}e^{-\beta\epsilon}$ we finally arrive at the effective Schrödinger equation

$$\left[-\frac{1}{2\beta^2\xi^2(1-r)^2a}\frac{d^2}{dy^2}+\frac{a}{4}[(1-r)^2y^2-1]^2\right]h(y)=\epsilon h(y) \quad , \tag{67}$$

where ξ is the width of the zero velocity soliton.

As expected (67) reduces to the differential equation obtained by KS in the limit $r \to 0$. The largest eigenvalue λ_0 of the integral equation corresponds to the ground-state energy of (67). With the change of variable $x=(1-r)y$, Eq. (67) reduces to

$$\left[-\frac{1}{2\beta^2 a\xi^2}\frac{d^2}{dx^2}+\frac{a}{4}(x^2-1)^2\right]h=\epsilon h \ . \tag{68}$$

The potential has two degenerate minima at $x=\pm 1$. For very low temperatures the effective mass $m^*=\beta^2 a\xi^2$ of the "particle" becomes very large so that the low-lying states are localized at the bottom of the wells and are essentially degenerate. This degeneracy is broken by tunneling across the barrier, which becomes increasingly more important as the temperature rises. On the other hand, at a fixed temperature the effective mass increases as r increases since $\xi \propto (1-r)^{-1}$ so that the tunneling becomes less important. In the limit $r \to 1$, $m^*=\beta^2\xi^2 a \to \infty$ and the ground state becomes degenerate. According to the traditional wisdom such a degeneracy is characteristic of an ordered phase. On the other hand, (68) would imply that the system is ordered at all temperatures as $r \to 1$. However, this cannot be true since at high enough temperature the system must be disordered. This question will be discussed in more detail in the next section where we treat the van der Waals's limit by an alternative method.

The ground-state energy can be obtained by expanding the potential around each minimum. These yield harmonic oscillation states at each well with doubly degenerate spectrum $E_n=(n+\frac{1}{2})\omega$, where $\omega=\sqrt{2}/\beta\xi$. The degeneracy is broken by tunneling across the barrier. A standard WKB treatment[5,20] yields for the ground-state energy

$$\epsilon_0=\frac{1}{\sqrt{2}\beta\xi}-\left[\frac{16}{\pi}\right]\left[\frac{a}{4}\right]\left[\frac{e}{\sqrt{2}\beta\xi a}\right]^{1/2}\exp\left[-\frac{2\sqrt{2}}{3}\beta\xi a\right] \ . \tag{69}$$

Since

$$\lambda_0=\left[\frac{2\pi}{\beta\xi^2(1-r)^2 a}\right]^{1/2}e^{-\beta\epsilon_0} \tag{70}$$

we have for the free energy per particle

$$\begin{aligned}\frac{F}{N}&=-\frac{1}{2\beta}\ln\left[\frac{2\pi}{\beta}\right]-\frac{1}{2\beta}\ln\frac{2\pi}{\beta\xi^2(1-r)^2 a}+\epsilon_0\\&=\frac{1}{N}F_{\text{ph}}+\frac{1}{N}F_{\text{tunn}}\end{aligned} \tag{71}$$

with

$$\frac{1}{N}F_{\text{ph}}=\frac{1}{\beta}\left[\frac{1}{\xi\sqrt{2}}+\ln\frac{\beta\xi(1-r)\sqrt{a}}{2\pi}\right] \tag{72}$$

and

$$\frac{1}{N}F_{\text{tunn}}=-\frac{1}{\beta}\left[\frac{4a}{\pi}\right]\left[\frac{e}{\sqrt{2}\beta\xi a}\right]^{1/2}\exp\left[-\frac{2\sqrt{2}}{3}\beta\xi a\right] \ . \tag{73}$$

If we neglect the σ corrections in Eq. (33) then

$$\frac{2\sqrt{2}}{3}\xi a=E_s$$

is the energy of a zero-velocity soliton. The tunneling term then becomes

$$-\frac{1}{\beta}\left[\frac{4a}{\pi}\right]\left[\frac{2e}{3\beta E_s}\right]^{1/2}e^{-\beta E_s} \ .$$

This is just the contribution of the solitons to the free energy which is seen to fall off as the soliton energy E_s increases, as is shown by KS. As $r \to 1$, $E_s \to \infty$ and this term vanishes. Similarly, from Appendix A we see that F_{ph} is nothing but the phonon free energy. Again, as $r \to 1$ the first term in (77) vanishes since $\xi \to \infty$. However, since $\xi(1-r)$ remains finite in the limit $r \to 1$, the second term gives a finite contributions to the free energy.

IV. VAN DER WAALS LIMIT: $r \to 1$

The behavior of the system in the limit the range of the interaction becomes infinite has been extensively studied in connection with Ising[14–16] and Potts's[17] models. As $r \to 1$, these models exhibit a continuous phase transition at a finite temperature T_c. Since Φ^4 model is similar to the Ising model we expect it to exhibit similar behavior. In what follows we study the van der Waals limit ($r \to 1$) of the model under consideration. The treatment presented here parallels those of Baker (Ising model) and Vishwanath and Meyer (Potts's model).

In the limit $r \to 1$, we rewrite (54) as

$$\begin{aligned}\lambda\Phi(y)&=\int_{-\infty}^{\infty}dy'\int_{-\infty}^{\infty}du\,\exp[-\beta W(u)+K(1-r)uy]\delta(y'-u-ry)\Phi(y') \ ,\\&=\int_{-\infty}^{\infty}du\,\exp[-\beta W(u)+K(1-r)uy]\Phi(u+ry) \ .\end{aligned} \tag{74}$$

A. $K=0$

In the special case, $K=0$, Eq. (74) can be solved exactly for arbitrary r. Putting $K=0$ in (74) we get

$$\lambda\Phi(y)=\int_{-\infty}^{\infty} du\, e^{-\beta W(u)}\Phi(u+ry) \ . \tag{75}$$

Let

$$\nu=\int_{-\infty}^{\infty} du\, e^{-\beta W(u)} \ . \tag{76}$$

Then the solutions are of the form

$$\Phi_{2p}(y)=\sum_{m=0}^{p} a_m y^{2m} \ , \tag{77}$$

$$\Phi_{2p+1}(y)=\sum_{m=0}^{p} b_m y^{2m+1} \ . \tag{78}$$

Substituting (77) and (78) in (75) and equating the coefficients of y^{2p} and y^{2p+1}, respectively, give the eigenvalues

$$\lambda_p=\nu r^p \ . \tag{79}$$

The coefficients a_m and b_m can be unambiguously determined by equating coefficients of y^m. This gives

$$\lambda_{2p}a_n=\sum_{m=n}^{p}\binom{2m}{2n} r^{2n}a_m F_{m-n} \ , \tag{80}$$

$$\lambda_{2p+1}b_n=\sum_{m=n}^{p}\binom{2m+1}{2n+1} r^{2n+1}b_m F_{m-n} \ , \tag{81}$$

where

$$F_{m-n}=\int_{-\infty}^{\infty} du\, e^{-\beta W(u)}u^{2m-2n} \ . \tag{82}$$

We remark here that as $r\to 1$, all the eigenvalues converge to $\lambda_0=\nu$ [Eq. (79)]. However, since $K=0$ means that there is no interaction between the particles, there is no phase transition implying that the largest eigenvalue should be nondegenerate. The apparent ambiguity can be resolved by noting that the limit $r\to 1$ should be taken only after $N\to\infty$, i.e., the thermodynamic limit is taken. The limit $r\to 1$ actually corresponds to[16] $r\to 1$, $r^N\to 0$, as $N\to\infty$. Thus the contribution to the partition function $p^N r^{Np}$ vanishes for any $p\neq 0$, so that only the $p=0$ state contributes.

B. Maximum eigenvalue for arbitrary K

Let us define $g(y)=\Phi(y/(1-r))$, then Eq. (74) becomes

$$\lambda g(y)=\int_{-\infty}^{\infty} du\, \exp[-\beta W(u)+Kuy] \times g((1-r)u+ry) \ . \tag{83}$$

The exponential $e^{-\beta W(u)}=\exp[-Ku^2-\beta\frac{1}{4}a \times (u^2-1)^2]$ ensures that contribution to the integral for $u \gg 1$ is minimal. In the limit $r\to 1$, we write

$$g((1-r)u+ry)\simeq g(y)+(1-r)(u-y)\frac{dg}{dy} \simeq g(y)e^{(u-y)q(y)} \ , \tag{84}$$

where $q(y)=(1-r)g'/g$. Then (83) becomes

$$\lambda=\int_{-\infty}^{\infty} du\, \exp[-\beta W(u)+Kuy+(u-y)q(y)] \ . \tag{85}$$

Since λ must be independent y, we set $d\lambda/dy=0$, which gives

$$[K+q'(y)]F'(Ky+q(y)) = [q(y)+yq'(y)]F(Ky+q(y)) \ , \tag{86}$$

where

$$F(\chi)=\int_{-\infty}^{\infty} \exp[-\beta W(u)+u\chi]\, du \ , \tag{87}$$

$$F'(\chi)=\int_{-\infty}^{\infty} \exp[-\beta W(u)+u\chi]u\, du \ . \tag{88}$$

Defining $G(\chi)=F'(\chi)/F(\chi)$, we can rewrite Eq. (86) as

$$q'(y)=\frac{KG(Ky+q(y))-q(y)}{y-G(Ky+q(y))} \ . \tag{89}$$

Since the eigenvalue is independent of y it suffices to evaluate the right-hand side of Eq. (85) for any particular y. Following Baker[16] we now note that $q'(y)=g'(y)/g(y)$ must be finite, so that if the denominator in (89) vanishes anywhere, the numerator must also. Thus, if

$$y=G(Ky+q(y)) \tag{90}$$

then

$$q(y)=KG(Ky+q(y)) \ . \tag{91}$$

Combining (90) and (91) we obtain

$$Z_0=2KG(Z_0) \ , \tag{92}$$

where $Z_0=Ky_0+q(y_0)$. Dividing (90) by (91) we also see that at this point $y=y_0$, $q(y_0)=Ky_0$, so that

$$\lambda=e^{-Z_0^2/4K}F(Z_0) \ . \tag{93}$$

The free energy per particle is then given by

$$-\beta f=\lim_{N\to\infty} N^{-1}(\ln Z_p+\ln Z_u)=\ln\left[\frac{2\pi}{\beta}\right]+\ln\lambda \ . \tag{94}$$

Using Eqs. (92)–(94) one then obtains for the internal energy and the specific heat per particle

$$U=\tfrac{1}{2}k_BT-Z_0^2/4K^4\ , \tag{95}$$

$$\frac{C_v}{k_B}=\frac{1}{2}+\frac{Z_0^2G'(Z_0)}{1-2KG'(Z_0)}\ . \tag{96}$$

To obtain an expression for the order parameter $\langle u\rangle=m$, we must include a term in $W(u)$ which describes the coupling to the external field h. Let

$$W(u)=W_0(u)-hu\ , \tag{97}$$

where the subscript stands for the zero-field quantities. From (87) it then follows that $G(Z)=G_0(Z+H)$, with $H=\beta h$. The magnetization is then given by

$$m=\frac{\partial}{\partial H}(-\beta f)=G(Z_0)=\frac{Z_0}{2K}\ . \tag{98}$$

Notice that (98) holds also for $H=0$. In this case a finite Z_0 implies the existence of a spontaneous order in the system.

In the absence of a field we have only to consider the function $G_0(Z)$. Since $F(Z)$ as defined by (87) is an even function, it follows that $G_0(Z)$ is an odd function of its argument. Recall that $\theta=a/J$. Then as $\theta\to\infty$, the only contributions in the integral in (87) come from $u=\pm 1$, i.e., the model reduces to the Ising model. Thus as $\theta\to\infty$, $F(Z)=\cosh Z$ and $G_0(Z)=\tanh Z$. For other values of θ, we have numerically evaluated $G_0(Z)$. Some typical curves are shown in Fig. 3. It is clear that $G_0(Z)$ is monotonic in Z and $G_0'(Z)$ decreases with increasing Z.

Since $G_0(Z)$ is odd $Z_0=0$ is a solution of Eq. (92). In the neighborhood of $Z=0$, $G_0(Z)$ can be expanded in a power series of form

$$G_0(Z)=b_0(K,\theta)Z-b_1(K,\theta)Z^3+\cdots\ , \tag{99}$$

where the coefficient $b_0,b_1>0$. If $2Kb_0<1$, then $G(Z)$ will never cross the line $y=Z/2K$, hence the only solution is at $Z_0=0$. This regime corresponds to the disordered or high-temperature phase of the system. For $2Kb_0>1$, however, there is another solution at $Z=Z_0\neq 0$, which corresponds to the ordered phase. The critical temperature is given by

$$2K_Cb_0(K_C,\theta)=1\ . \tag{100}$$

K_C is in general a function of θ. The thermodynamic functions can be obtained by solving Eq. (92) numerically for Z_0.

For T close to T_c ($T<T_c$) Z_0 is small, using (99) up to the cubic term we can solve for Z_0:

$$Z_0^2\simeq\frac{1}{b}\left[b_0(K,\theta)-\frac{1}{2K}\right]\ . \tag{101}$$

To calculate b_0 and b_1 we express $F(x)$ [Eq. (87)]

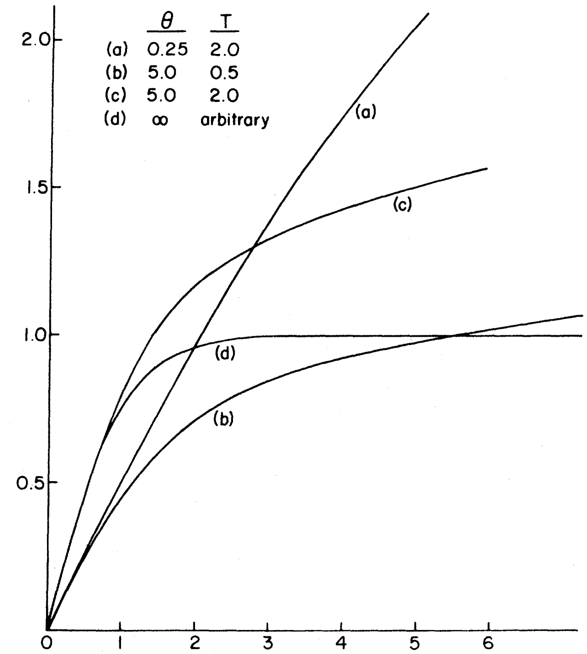

FIG. 3. Function $G(Z)$ for $Z>0$ and for various values of $\theta=a/J$ and temperatures $T=K^{-1}$.

as a power series in x

$$F(x)=\sum_{n=0}^{\infty}\frac{a_nx^{2n}}{2n!}\ , \tag{102}$$

where

$$a_n=\int_{-\infty}^{\infty}dy\,y^{2n}\exp\left[-\frac{K}{2}(2-\theta)y^2-\frac{K\theta}{4}y^4\right]\ . \tag{103}$$

Integrating by parts once, we obtain

$$a_{n+2}=-\frac{2-\theta}{\theta}a_{n+1}+\frac{2n+1}{K\theta}a_n\ . \tag{104}$$

Using (102) and (104) and the defining relation

$$G(x)=\frac{F'(x)}{F(x)}=\sum_n b_nx^{2n+1}(-1)^n$$

it can be shown that

$$b_0=\frac{a_1}{a_0}=\frac{\int dy\,y^2\exp\left[-\frac{K}{2}(2-\theta)y^2-\frac{K\theta}{4}y^4\right]}{\int dy\,\exp\left[-\frac{K}{2}(2-\theta)y^2-\frac{K\theta}{4}y^4\right]}\ , \tag{105}$$

$$b_1=\frac{1}{G}\left[\frac{1}{K\theta}-\frac{2-\theta}{\theta}b_0-3b_0^2\right]\ . \tag{106}$$

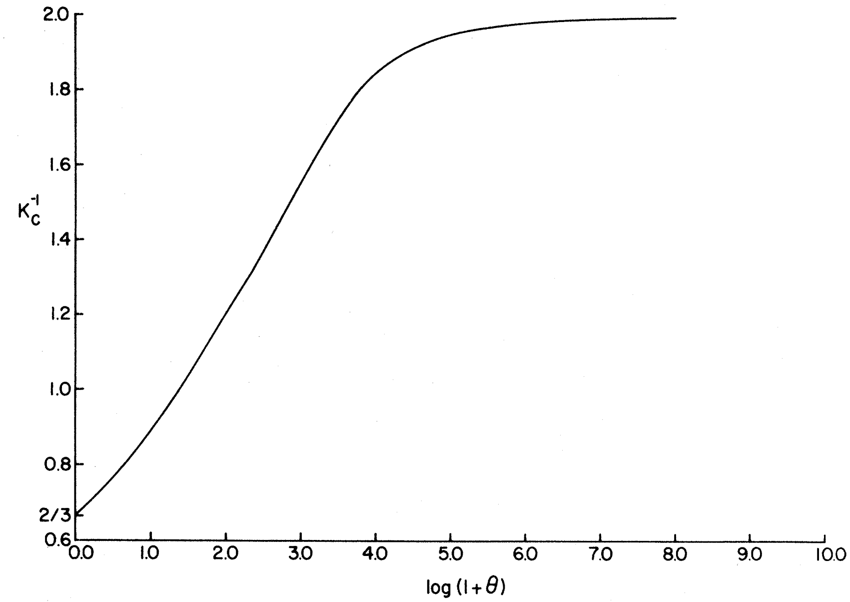

FIG. 4. Critical temperature K_C^{-1} as a function of $\ln(1+\theta)$.

In the Ising limit $\theta \to \infty$, $b_0 = 1$, which gives for critical "temperature" $K_C^{-1} = 2$, in agreement with Baker. As $\theta \to 0$, on the other hand, the quartic term in (105) vanishes and doing the Gaussian integrals we obtain $K_C^{-1} = \frac{2}{3}$. Between these two limits K_C^{-1} varies smoothly with θ, as is shown in Fig. 4.

Expanding b_0, b_1 about K_C, we see that the magnetization per particle diverges as

$$m = Z_0 \sim (T_c - T)^{1/2} \ . \tag{107}$$

Using (99), (100), (105), and (106) in (96) we obtain for the specific heat at T_c

$$\frac{C_v}{k_B} = \frac{1}{2} + \frac{1}{1 - 2K_C/3} \ . \tag{108}$$

The above results agree with Baker[16] in the Ising limit. From (108) it is apparent that the height of the specific-heat maximum increases as θ decreases, diverging at $\theta \to 0$.

V. DISCUSSION AND CONCLUSIONS

In conclusion, we have studied the effect of long-range interactions on nonlinear solitonlike excitations. The particular model chosen was the one-dimensional strongly anharmonic u^4 model used to study displacive phase transition. The interaction between displacement fields at different points were taken to fall off exponentially with separation. The virtue of this particular interaction is that the range of interaction γ^{-1} can be varied continuously. Whereas in the short-range limit the model exhibits solitonlike excitations which play an important role in the low-temperature thermodynamics and the dynamics of the system, as the range becomes infinite the model undergoes a second-order phase transition. By studying the equations of motion, we have found closed-form expressions for low-velocity single-soliton solutions. These solutions reduce to the well-known kink solutions in the short-range limit. However, as the range of interaction is increased the width and the energy of the solitons were both found to increase indefinitely with the range so that these solitons could no longer be considered as low-temperature excitations. This is expected since single solitons tend to destroy long-range order, and therefore in the limit of infinite range they must become energetically less favorable for the sytem to support. On the other hand, soliton-antisoliton pairs can still be considered as low-energy excitations. Unfortunately, for the u^4 model no multisoliton solution has been obtained even in the short-range limit.

By using a novel mathematical transformation we have converted the problem of calculating the partition function into an equivalent nearest-neighbor problem. The partition function is evaluated by the familiar transfer-integral technique. When the range of the interaction is small it is seen that the solitons play an important role at low temperatures. However, as the range is increased their contribution to the low-temperature free energy is found to vanish. In the infinite-range limit the system, as expected, undergoes a continuous phase transition. The critical properties are identical to a van der Waals model as were discussed by Baker.[16]

An important feature in these systems is the appearance of a central peak in the dynamic response function $S(q,\omega)$. Krumhansl and Schrieffer[5] have shown that this peak is related to the motion of the domain walls; in particular, they have shown that the height of the peak increases as e^{E_s/k_BT}. Physically, the central peak corresponds to the slow oscillation of clusters of ordered atoms reflecting the existence of short-range order in the system. This short-range order persists (above $T=0$) up to temperature $k_BT^* \sim E_s$. This means in our case that the T^* increases with the range of the interaction.

Finally, we remark that it would be very interesting to study the role of soliton-antisoliton pairs since they do not destroy the long-range order. One possible model for which this might be feasible is the sine-Gordon model since in this case multisoliton solutions are known in the short-range limit. However, we have not yet succeeded in obtaining closed-form soliton solutions for the long-range sine-Gordon model.

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APPENDIX A: STATISTICAL MECHANICS OF PHONONS

To calculate the contribution of the phonons to the low-temperature free energy we use the formula

$$\beta F_{\rm ph} = \int_0^\pi dq \left(\frac{dn}{dq}\right) \ln(1-e^{\beta\hbar\omega}) \simeq \frac{N}{\pi}\int_0^\pi dq\, \ln\beta\hbar\omega \tag{A1}$$

in the classical limit $\beta << \hbar$. Using the dispersion relation

$$\omega^2 = 2a + \frac{J(1+r)q^2}{rq^2+(1-r)^2}$$

we then have

$$\beta F_{\rm ph} = \frac{N}{2}\left[\ln\beta^2\hbar^2\left(2a+\frac{J(1+r)\pi^2}{r\pi^2+(1-r)^2}\right) + \frac{2}{\pi}\left(\frac{2a(1-r)^2}{2ar+J(1+r)}\right)^{1/2}\tan^{-1}\pi\left(\frac{2ar+J(1+r)}{2a(1+r)^2}\right)^{1/2} - \frac{2}{\pi}\frac{1-r}{\sqrt{r}}\tan^{-1}\frac{\pi\sqrt{r}}{1-r}\right] . \tag{A2}$$

In the limit $r\rightarrow 0$, we shall write

$$2a+\frac{J(1+r)\pi^2}{r\pi^2+(1-r)^2} \simeq 2a + \frac{\pi^2\xi^2 a(1-r)^2+ar\pi^2}{r\pi^2+(1-r)^2}$$

$$\simeq \xi^2 a\pi^2(1-r)^2 ,$$

$$\frac{1-r}{\sqrt{r}}\tan^{-1}\frac{\pi\sqrt{r}}{1-r} \simeq \pi ,$$

$$\frac{2a(1-r)^2}{2ar+J(1+r)} \simeq \frac{2}{\xi^2} ,$$

$$\tan^{-1}\pi\left(\frac{2ar+J(1+r)}{2a(1-r)^2}\right)^{1/2} \simeq \frac{\pi}{2} .$$

In the approximation above we have assumed that $J >> a$, i.e., $\xi >> 1$. The phonon free energy then becomes (with $\hbar=1$)

$$\beta F_{\rm ph} \simeq N\left[\ln\beta\xi\pi\sqrt{a}\,(1-r) + \frac{1}{2}\left(\frac{2}{\xi^2}\right)^{1/2} - 1\right]$$

$$= N\left(\frac{1}{\xi\sqrt{2}} + \ln\frac{\beta\xi\pi\sqrt{a}\,(1-r)}{e}\right) \tag{A3}$$

which is essentially the same as Eq. (72) apart from a factor of order unity in the logarithm.

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