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Statistical-mechanical treatment of kinks in a one-dimensional model for displacive phase transitions

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We have studied the equilibrium properties of a one-dimensional model system whose displacement field Hamiltonian is anharmonic and is representative of those used in the study of structural phase transitions. For low temperatures, a new set of intrinsically nonlinear configurations which are not accessible via perturbation theory play an important role. These "kink" configurations are solutions of the classical field equations and represent clusters of locally ordered regions observed in computer simulations. We have successfully incorporated the multikink configurations in our analysis and have carried out an approximate calculation of the partition function and the static structure factor. We find that the low-temperature and small-wave-number behavior of the system is dominated by the kink degrees of freedom. At higher temperatures and wave numbers the system is "phonon dominated."

I. INTRODUCTION

We have studied the static and dynamic properties of a one-dimensional model field theory whose displacement field Hamiltonian is anharmonic and is representative of those used in the study of structural phase transitions.[1,2] Computer simulations carried out for this model independently by Schneider and Stoll[3] and Koehler *et al.*[4] show the existence of clusters of locally ordered regions which generate a "central peak" for small wave numbers k and low temperatures in the dynamic structure factor $S(k,\omega)$. These locally ordered regions also lead to a damping and "softening" in the phonon frequency as $T\to 0$ and $k\to 0$.

A formal analysis of our model based on self-consistent perturbation theory can describe the damping of the phonons. It gives no information, however, about the softening of the phonons and the origin of the central peak. Furthermore, as one expects, perturbation theory fails close to the transition temperature $T_c = 0$ as the displacements of atoms relative to the reference lattice become very large and highly correlated. It is consequently important at low temperatures to treat a new set of intrinsically nonlinear field configurations not accessible via perturbation theory. These kink configurations are solutions of the classical field equations and represent the clusters of locally ordered regions observed in the computer simulations.

In this paper we develop new theoretical methods for treating these local-field configurations. Using these techniques, we will show in a second paper how one can theoretically account for the central peak in the dynamic structure factor as well as the damping and softening of the phonons for small wave numbers and low temperatures. Before discussing these methods, however, we want to indicate how similar "excitation" are entering into other areas of physics and how our problem interfaces with them.

The importance of local-field configurations in understanding the properties of large classes of field theories is becoming increasingly evident. These local configurations are referred to in various contexts as solitons, instantons, droplets, domains, vortices, or the general term we shall use, pseudoparticles. These pseudoparticles lead to qualitative changes in the physics of a problem from that predicted by the conventional perturbative treatment of the same problem. In this sense these configurations are generated by intrinsically nonlinear processes missed by perturbation-theory treatments.

Pseudoparticles appear to be important in three rather different physical situations. It is well known from the work of Langer[5] (and others[6-8]) that local-field configurations (like droplets) lead to nucleation in metastable systems. These droplets drive the system to tunnel from a false vacuum or metastable configuration to the true vacuum or equilibrium configuration. A second and related context in which these configurations become important involves the method of asymptotic estimates of perturbation theory expansions due to Lipatov,[9] and developed by Brézin, LeGuillou, Zinn-Justin, and collaborators.[10-12] In this case the structure of a perturbation-series expansion (its asymptotic nature) is controlled by instabilities that exist as one analytically continues the system to unphysical values of the coupling in which one is expanding. These instabilities are very closely related to those which occur in the case of metastability and therefore are characterized by local-

field configurations like droplets. In the language of Brézin, Le Guillou, and Zinn-Justin[11] "complex pseudoparticles" with associated finite action indicate that a perturbation theory is "Borel summable" and therefore useful. Finally there is a third situation where pseudoparticles play a significant role. This is in the case of systems with degenerate vacuums. Ordinarily when one has a system with degenerate vacuums and one lowers the temperature, spontaneous symmetry breaking will occur. This is the standard behavior in $O(n)$ symmetric φ^4 field theories for dimensionality greater than 2. In lower-dimensional systems, however, there can exist "real" pseudoparticles which act to restore the symmetry.[11] They serve as a mechanism for tunneling between the degenerate states. The existence of these real pseudoparticles has been shown by Brézin, LeGuillou, and Zinn-Justin[12] to lead to non-Borel summability of the associated perturbation theory. This is manifested, characteristically, in the appearance of terms like $e^{-A/g}$ in physical quantities, where g is the nonlinear coupling constant and A is a constant.

Within the context of stable systems where pseudoparticles are important, there appear to be two rather different subclasses of systems. These classes are distinguished by the nature of the interaction between pseudoparticles and the energy needed to create an isolated pseudoparticle. In the case of the planar or x-y model in two dimensions, the relevant pseudoparticles are vortices which interact via a long-range potential, and the energy to create a vortex increases logarithmically with the size of the system.[13] This has the consequence that at low temperature vortices appear only in pairs. At high temperatures, however, the vortices can dissociate leading to a metal-insulator-type of phase transition.[14] The second subclass of systems, including that studied in this paper, are those with real pseudoparticles with a finite "creation" energy and short-range interaction between the pseudoparticles.[15]

In high-energy theory there has been considerable study of pseudoparticles. In most of these calculations[16] it is assumed that there is exactly one pseudoparticle and one contructs a perturbation theory about this single pseudoparticle. In many solid-state contexts it is unphysical to talk about just one pseudoparticle or even a constant number of pseudoparticles. Landau's famous argument[17] concerning the absence of phase transitions in one dimension is built on the existence of a finite density of kinks in a system at low temperatures. Indeed in all of the situations mentioned above, stable and unstable, it is important to investigate the role of multipseudoparticle configurations. In the case of the planar model, only multiple-vortex excitations (bound pairs) are energetically allowed for low temperatures.[18] In the case of metastable systems it is clear from the work of Langer[5] and Callen and Coleman[7] that one must treat multipseudoparticle configurations if one is to produce the correct linked cluster or volume dependences of physical systems.

In the problem we are interested in here, essentially a quantum-mechanical oscillator with a double-well potential, it is clear from the work of Krumhansl[2] and Schrieffer and Polyakov[19] that multikink configurations are essential for an understanding of the low-temperature properties of the system. Heretofore, however, the analysis of this problem has been essentially heuristic. Our objective has been to develop a systematic method for treating multikink configurations. Thus we develop a series of transformations which take us from an initial problem of a field theory with a degenerate double-well potential to a theory coupling kinks and a field in a single-well potential.

There are various advantages and disadvantages in working on a one-dimensional system. The advantages are primarily technical in nature. (i) There are no renormalization problems in one dimension. (ii) We can evaluate the static properties of our model explicitly since we can do one-dimensional functional integrals exactly.[2,20] Thus we have a check on our approximation methods. This is, however, not true for the dynamic properties of our model. (iii) Finally we know much more about pseudoparticle solutions in one dimension than we do for higher dimensions.

The main disadvantage of working in one dimension is that one is skeptical about the generalization of the results to higher dimensions. We note, for example, that in one dimension the temperature where the density of kinks goes to zero and the "phase transition" temperature T_c are the same. This will clearly not hold in higher dimensions. It does appear from molecular dynamics[1] that there are important contributions to the structure factor due to "domains" in higher dimensions. It is not at all clear, however, how one can introduce, in a clean manner, "finite action" pseudoparticles in higher dimension which look like domains and are approximate solutions of the classical-field equations. It is also not clear that the central peak we find in one dimension has anything to do with the central peak found in scatttering experiments.[21]

In Sec. II of this paper we define the problem of interest. In Secs. III, IV, and V we discuss what is known about the problem using conventional perturbation theory and computer analysis. We introduce our multikink approach in Sec. VI. We use this approach in Sec. VII to analyze the thermody-

namic properties of our model. We conclude with a short discussion in Sec. VIII.

II. DEVELOPMENT OF THE MODEL

We will consider a continuum model[1] representing a set of oscillators in an anharmonic double-well potential

$$A\{\varphi\}=\int_{-L}^{+L} dx\left[\frac{1}{2}\left(\frac{d\varphi}{dx}\right)^2+U\{\varphi\}\right], \tag{2.1}$$

$$U\{\varphi\}=-\tfrac{1}{2}\kappa^2\varphi^2(x)+\tfrac{1}{4}u\varphi^4(x), \tag{2.2}$$

where our system has a length $2L=V$ and $\varphi(x)$ is a displacement field. κ and u are positive constants taken as parameters in our model.

We will be interested in calculating the thermodynamic properties of our system via the partition function

$$Z_\varphi=\int \mathfrak{D}\varphi\, e^{-\beta A\{\varphi\}}, \tag{2.3}$$

where $\beta=(k_BT)^{-1}$ is the inverse temperature. Our definition of the functional integral in Eq. (2.3) is given by

$$Z_\varphi=\lim_{N\to\infty}\lim_{l\to 0}\prod_{i=1}^{N}\int_{-\infty}^{\infty}\frac{d\phi_i}{(2\pi l)^{1/2}}\, e^{-\beta A\{\varphi_i\}}, \tag{2.4}$$

where the discrete version of A is

$$A\{\varphi_i\}=l\sum_{i=1}^{N}\left(\frac{(\varphi_{i+1}-\varphi_i)^2}{2l^2}-\frac{\kappa^2\varphi_i^2}{2}+\frac{u}{4}\varphi_i^4\right). \tag{2.5}$$

In the limiting process above we require that the product $Nl=V$ be held constant and that the fields are periodic $\varphi_{i+N}=\varphi_i$. With this convention we have the result for Gaussian integrals

$$Z_G=\int \mathfrak{D}\varphi\, e^{-\beta A_G\{\varphi\}}=e^{-\beta V\omega/2}, \tag{2.6}$$

where

$$A_G=\frac{1}{2}\int_{-L}^{L} dx\left[\left(\frac{d\varphi}{dx}\right)^2+\omega^2\varphi^2(x)\right]. \tag{2.7}$$

We will also be interested in the static structure factor

$$S(x-x')=\frac{1}{Z_\varphi}\int \mathfrak{D}\varphi e^{-\beta A[\varphi]}\varphi(x)\varphi(x'), \tag{2.8}$$

and its Fourier transform

$$S(k)=\int d(x-x')e^{ik(x-x')}S(x-x'), \tag{2.9}$$

which has been calculated in molecular dynamics simulations. The parameters of our model have the dimensions (E, energy; L, length):

$$\beta\ [E^{-1}],\quad \kappa\ [L^{-1}],$$

$$\varphi\ [EL]^{1/2},\quad u\ [E^{-1}L^{-3}]. \tag{2.10}$$

It is clear that the dimensionless coupling constant in this problem is

$$\epsilon=u/\beta\kappa^3, \tag{2.11}$$

which, for arbitrary u, is small at low temperatures. In calculating the free energy

$$F=-\beta^{-1}\ln Z\varphi, \tag{2.12}$$

it is clear that in the thermodynamic limit

$$F=-\beta^{-1}(\kappa V)f(\epsilon),$$

where f is a function of ϵ alone. This simple scaling argument holds because we do not need to introduce an ultraviolet cutoff in this one-dimensional theory.

In Secs. III–V we will discuss what we can learn about our model using a variety of techniques. In most of these sections the work we discuss is not our own, but we include it here since it is important to understand why one has to introduce special methods if one is to understand the time- and space-dependent correlations in this sytem. We will also try to draw out the differences between this model and apparently similar models where direct methods work to explain the statistical-mechanical properties.

III. IDEAS FROM PERTURBATION THEORY

Let us investigate in this section what we can learn about our "simple" one-dimensional field theory using a direct perturbation theory analysis in the quartic coupling u. Of course one cannot proceed directly because the coefficient of the quadratic term in the potential $U\{\varphi\}$ is negative. Consequently the zero-order propagator in a direct perturbation-series expansion is given by

$$G(q)=(q^2-\kappa^2)^{-1}, \tag{3.1}$$

which is clearly unacceptable since the pole at $q=\kappa$ is unphysical. We can circumvent this difficulty through the usual shifting procedure that is used to treat Ginzburg-Landau theories below a conventional critical point. In this case one recognizes that at low temperatures the oscillators want to sit at the bottom of one of the double wells. We keep in mind that in two and greater dimensions the symmetry between the wells will be spontaneously broken and we made the shift

$$\varphi(x)=\langle\varphi\rangle+\chi(x), \tag{3.2}$$

where $\langle\varphi\rangle$ is the spontaneously generated nonzero value for the field. In the one-dimensional case

the symmetry cannot be broken, $\langle\varphi\rangle = 0$, but we can choose to ignore this "small" point and expand about $\varphi(x) = +\kappa/\sqrt{u} + \chi(x)$ (where $\kappa\sqrt{u}$ is the value of φ at the bottom of one of the wells) anyway. We then obtain the new action

$$A\left(\frac{\kappa}{\sqrt{u}}+\chi\right) = E_{\text{vac}} + \int_{-L}^{L} dx \left[\frac{1}{2}\left(\frac{d\chi}{dx}\right)^2 + \kappa^2\chi^2 + \kappa\sqrt{u}\chi^3 + \frac{u}{4}\chi^4\right], \quad (3.3)$$

where

$$E_{\text{vac}} = -\kappa^4 V/4u \quad (3.4)$$

is the vacuum energy. The zero-order in u propagator is

$$G^0(q) = (q^2 + 2\kappa^2)^{-1}, \quad (3.5)$$

and we can treat the cubic and quartic terms in χ as perturbations and calculate the free energy as a power series in the dimensionless coupling ϵ:

$$f(\epsilon) = \sum_{n=0}^{\infty} f_n \epsilon^n. \quad (3.6)$$

We list in Table I the first few terms in this expansion. It is abundantly clear that this expansion is of dubious merit for finite coupling ϵ. Recently, however, techniques have been developed for analyzing the nature of such obviously asymptotic perturbation-expansion series and for finding ways of extracting useful information about observables for finite values of the coupling. It is useful for us to use these new ideas in order to understand the nature of the perturbation series discussed above.

Let us begin the discussion with an analysis of a model more general than that defined in Sec. II. Let us assume that $U\{\varphi\}$ is a polynomial of the form

$$U\{\varphi\} = \frac{1}{g^2} W\{g\varphi\}, \quad (3.7)$$

where $\varphi = 0$ is a minimum of the potential and we normalize about $\varphi = 0$ such that

$$W\{\varphi\} = \tfrac{1}{2}\varphi^2 + O(\varphi^3), \quad (3.8)$$

g is the coupling constant and the difference $(1/g^2)W\{g\varphi\} - \frac{1}{2}\varphi^2$ is treated as a perturbation. The second term in Eq. (3.3) can be written in this form if we choose $\kappa^2 = 1, u = g^2$. One can now go ahead and carry out a direct perturbation theory expansion for the free energy

$$F = -\beta^{-1}\ln Z_\varphi = \sum_{K=0}^{\infty} F_K g^{2K}. \quad (3.9)$$

It is, of course, well known how to extract the lowest-order terms in F_K using Feynman graph methods.[23] Recently, however, using methods due to Lipatov,[9] Brézin, Le Guillou, and Zinn-Justin[10-12] have shown how one can compute F_K for large K. To a large extent the nature of the perturbation-series expansion is controlled by the location of stationary points of the action $A\{\varphi\}$ in function space. Thus, for large β, small ϵ, one expects the functional integral Z_φ to be dominated by those portions of function space satisfying

$$\delta A\{\varphi\}/\delta\varphi(x) = 0. \quad (3.10)$$

This is, of course, in simplest terms a generalized steepest descent argument.[24] Using our form for the action (2.1) we obtain from the variational condition the Euler-Lagrange equation

$$\frac{d^2\varphi_c(x)}{dx^2} = U'\{\varphi_c\}. \quad (3.11)$$

If we write $U\{\varphi\} = -V\{\varphi\}$ we see that this reduces to Newton's law if we identify φ_c with position and x with time. We are all familiar with the method for constructing a general solution to Newton's law in one dimension. The "energy"

$$E = \frac{1}{2}\left(\frac{d\varphi_c}{dx}\right)^2 + V\{\varphi_c\} \quad (3.12)$$

is a constant of the motion so we can solve for

$$\frac{d\varphi_c(x)}{dx} = \pm\{2[E - V(x)]\}^{1/2}. \quad (3.13)$$

If φ_c^0 is a turning point satisfying

$$E = V\{\varphi_c^0\}, \quad (3.14)$$

then we can integrate to obtain

$$x - x_0 = \pm\int_{\varphi_c^0}^{\varphi_c} \frac{dy}{\{2[E - V(y)]\}^{1/2}}, \quad (3.15)$$

where x_0 is a constant of integration. It is useful to note that the action A corresponding to this classical solution is

$$A\{\varphi_c\} = \int_{-L}^{L} dx\left[\frac{1}{2}\left(\frac{d\varphi_c}{dx}\right)^2 + U\{\varphi_c\}\right] = VE + 2\int_{-L}^{L} dx\, U\{\varphi_c\}. \quad (3.16)$$

TABLE I. First six terms of the perturbation-series expansion of the free energy.

n	f_n
0	−0.707
1	+0.25
2	0.199
3	0.348
4	0.865
5	2.693

Brézin *et al.*[10-12] have found that the asymptotic behavior of F is controlled by the existence of solutions $\varphi_c(x)$ of (3.11) that are periodic $[\varphi_c(x) = \varphi_c(x+V)]$ and which give a finite nonzero value for A as $L \to \infty$ ($A\{\varphi_c\}$ finite). In order for $A\{\varphi_c\}$ to be finite it is clear that $\varphi_c(x)$ must be localized in space[25] and must correspond to an energy $E[V]$ that goes to zero faster than $1/V$ as $V \to \infty$. Then

$$\lim_{L\to\infty} A\{\varphi_c\} = 2\int_{-\infty}^{\infty} dx\, U\{\varphi_c(x)\} \tag{3.17}$$

is finite. There are two main classes of potentials of interest. The first class is characterized by the potential in Fig. 1(a). The absolute minimum of $U_1\{\varphi\}$ is at $\varphi = 0$. If we consider $V_1\{\varphi\} = -U_1$ in Fig. 1(b) we see that the only periodic solution is trivial: $\varphi = 0$; this gives $A\{0\} = 0$ and does not control the convergence of the perturbation theory. Thus there is no "instantonic" solution of the equation of motion for the physical values of the parameters of the theory (β, κ, u). This is, from the point of view of perturbation theory, a desirable feature. In the last analysis an instanton represents an instability in a problem. In the case above there is no instability for the physical values of the parameters. We expect that the "nearest" instability corresponding to unphysical values of the parameters of the theory will control the convergence of the perturbation theory. Let us specialize the discussion to the simple case

$$U_0\{\varphi, g\} = \tfrac{1}{2}\varphi^2 + g^2\varphi^4 . \tag{3.18}$$

This is a single-well potential and clearly is an example where there is no instanton. If we analytically continue U_0 onto the complex g plane, then we see that

$$U_0\{\varphi, i\bar{g}\} = \tfrac{1}{2}\varphi^2 - \bar{g}^2\varphi^4 \tag{3.18a}$$

is of the form shown in Fig. 2(a).

The "potential" V shown in Fig. 2(b) leads to an instantonic solution. This corresponds to a solution that starts at $\varphi = 0$ at $x \to -\infty$, raises to $\varphi = \varphi_0$ at some position $x = x_0$ and then returns to $\varphi = 0$ as $x \to +\infty$. The zero-energy solution corresponding to this instanton can be obtained directly from Eq. (3.15). The turning point $\varphi_c^0 = \pm 1/(2\bar{g})$ is determined by the condition $E = V(\varphi_c^0) = 0$. We obtain via direct integration that

$$x - x_0 = -\ln\left(\frac{1 + [1 - (\varphi/\varphi_0)^2]^{1/2}}{\varphi/\varphi_0}\right), \tag{3.19}$$

which we can easily solve to obtain

$$\varphi = \varphi_0/\cosh(x - x_0) . \tag{3.20}$$

This instability on the negative $u = g^2$ axis characterizes the nature of the asymptotic perturbation series for positive u. In particular Brézin, Le

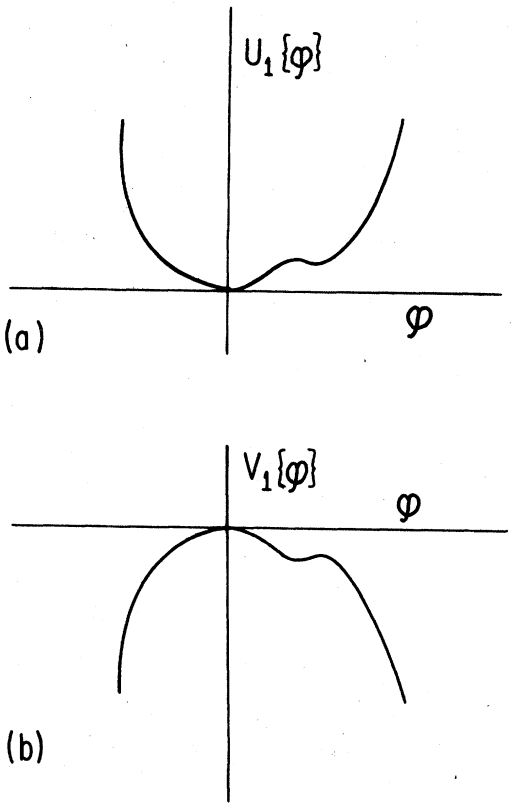

FIG. 1. (a) Potential $U_1(\varphi)$ vs φ with an absolute minima at $\varphi = 0$. (b) Potential $V_1(\varphi) = -U(\varphi)$ vs φ.

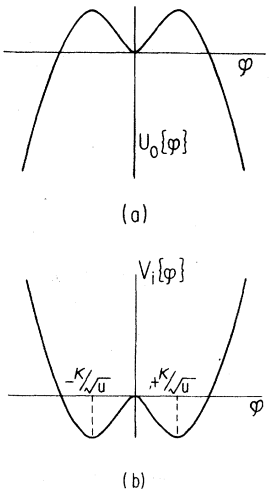

FIG. 2. (a) Symmetric potential with minimum at $\varphi = 0$ and two humps symmetrically located at $\varphi^0{}_c = \pm 1/(2\bar{g})$. (b) Symmetric double-well potential with minima located at $\varphi_c^0 = \pm\kappa/\sqrt{u}$.

Gulliou, and Zinn-Justin[10-12] have shown that the free energy in this case has an expansion

$$F(g)=\sum_{K=0}^{\infty} F_K g^{2K}, \tag{3.21}$$

where

$$F_K=\frac{-K!(-3)^K}{\sqrt{K}}\frac{6}{\pi^{3/2}}\left[1+O\left(\frac{1}{K}\right)\right]. \tag{3.22}$$

This expansion is clearly asymptotic. However, because of the $K!$ and the oscillating sign with K, it appears useful to perform a Borel transformation.[26] Write

$$F(g)=\sum_{K=0}^{\infty} g^{2K}\frac{F_K}{K!}\int_0^{\infty} dt\, t^K e^{-t}$$

$$=\int_0^{\infty} dt\, e^{-t} G(tg), \tag{3.21a}$$

where the Borel transform

$$G(z)=\sum_{K=0}^{\infty}\frac{F_K}{K!}Z^K \tag{3.23}$$

is analytic on the real positive axis. Suppose one then uses the first six terms in the expansion for $G(z)$ to determine a [3,3] Padé approximate. One can then insert this approximate G into (3.22) and do the integral over t. The result for $g=0.5$ calculated in this manner differs from the "exact" result[27] by only 10^{-3}.

An important and by now much studied problem is where the potential of interest is of the form given by U_0 as shown in Fig. 2(a). In this case one is interested in a metastable system where the metastable state corresponds to the local minimum at the origin. It is clear from the argument above that an instanton exists for the physical values of the parameters of the theory. Consequently the associated perturbation theory can be shown to be non-Borel summable. This is, of course, expected since the system will eventually tunnel to the absolute vacuum and this instability—a tunneling phenomenon—will lead to a breakdown of any perturbative approach. Langer[5] showed, however, how one could proceed in this case. The basic idea is to expand about the existing instanton. In this case one finds that there is a contribution to the free energy of the form

$$\exp(-A\{\varphi_c\})=\exp(-\text{const}/g^2),$$

which is clearly nonanalytic in the coupling constant. It is also found that the unstable nature of the system leads to an imaginary part to the free energy which one can associate with the lifetime of the metastable state. An interesting recent development[28] is that once one has properly expanded about the instanton the resulting perturbation expansion using the new action will be Borel summable. This follows from the fact that only a complex instanton exists for this new action $A'\{\chi\}=A\{\varphi_c+\chi\}-A\{\varphi_c\}$.

This progress on stable and metastable systems is encouraging and stimulates one to think that these ideas can be used to treat our degenerate double-well problem. Let us therefore return to the model defined by Eqs. (2.1) and (2.2). For low temperatures and large β we again expect that the dominant contributions to Z_φ will be from those field configurations $\varphi_c(x)$ which minimize $A\{\varphi\}$:

$$\left.\frac{\delta A}{\delta\varphi(x)}\right|_{\varphi=\varphi_c}=0=-\frac{d^2}{dx^2}\varphi_c(x)-\kappa^2\varphi_c(x)+u\varphi_c^3(x). \tag{3.24}$$

We discuss first the uniform solutions

$$\varphi_c^0=\pm\kappa/\sqrt{u},\,0. \tag{3.25}$$

The solutions $\varphi_c^0=\pm\kappa/\sqrt{u}$ are the usual mean-field symmetry breaking solutions. We know of course that these solutions are not stable[17] in finite temperature in a one-dimensional system due to tunneling. If we compute the "energy" corresponding to these solutions we obtain

$$A(0)=0, \tag{3.26}$$

$$A\left(\pm\frac{\kappa}{\sqrt{u}}\right)=-\frac{\kappa^4 V}{4u}=E_{\text{vac}}. \tag{3.27}$$

The broken symmetry state has the lowest energy. The solution $\varphi_c=0$ gives an energy that is very large compared to the energy associated with the symmetry-breaking solution. Since the configuration where all of the oscillators sit in one well is not thermodynamically stable at finite temperature there must be a low-lying excitation which is associated with this instability. We expect that this tunneling instability, which corresponds to the system switching from one vacuum state to the other, will be related to the instantonic instabilities we discussed in Sec. II.

In this case we are looking for solutions connecting the vacuum $+\kappa/\sqrt{u}$ and $-\kappa/\sqrt{u}$. For definiteness assume as $x\to-\infty$, $\varphi_c^0=+\kappa/\sqrt{u}$ and as $x\to-\infty$, $\varphi_c^0=-\kappa/\sqrt{u}$ and there is some finite transition region. The appropriate solutions are given by Eqs. (3.14) and (3.15) with $\varphi_c^0=\kappa/\sqrt{u}$. The energy in this case is nonzero,

$$E=V\{\varphi_c^0\}=-E_{\text{vac}}, \tag{3.28}$$

and the solution to the field equation is given by

$$x-x_0=\pm\int_0^{\varphi}\frac{dy}{\{2(E+U[y])\}^{1/2}}$$

$$= \pm\frac{\sqrt{2}}{\kappa}\int_0^{\varphi/\varphi_0}\frac{dz}{1-z^2}$$

$$= \pm(\sqrt{2}/\kappa)\tanh^{-1}(\varphi/\varphi_0)\,, \qquad (3.29)$$

where x_0 is the point where $\varphi = 0$. We then have the solution shown in Fig. 3,

$$\varphi(x) = \pm(\kappa/\sqrt{u})\tanh\left[\frac{\kappa}{\sqrt{2}}(x-x_0)\right]\,. \qquad (3.30)$$

These solutions connect the two degenerate vacua and look very much like the kinklike objects observed in computer simulations (see Sec. V). We also note that these kinks are reminiscent of the surface profile in the Van der Waals theory of a liquid-gas interface.[29] We can have a physical picture of a kink by noticing that the potential $V\{\varphi\}$ is a double-well potential [Fig. 2(b)], minima being at $\pm\kappa/\sqrt{u}$ and maxima at the origin. At low temperatures, the atoms will tend to sit in either of the wells. This situation corresponds to the symmetry breaking solution $\varphi_c = \pm\kappa/\sqrt{u}$. When some of the atoms flip from one well to another, we obtain a kink and so on. This has been schematically shown in Fig. 4. The "energy" of a kink configuration can be obtained directly from (3.16) as

$$A\{\varphi_0\} = -\kappa^4 V/4u + E_K\,, \qquad (3.31)$$

where

$$E_K = \frac{1}{2}\int dx\left[\left(\frac{\partial\varphi_0}{\partial x}\right)^2 - \kappa^2\varphi_0^2 + \frac{u}{2}\varphi_0^4 + \frac{\kappa^4}{2u}\right]$$

$$= \tfrac{2}{3}\sqrt{2}\,\kappa^3/u \qquad (3.32)$$

is the "kink" energy associated with the localized tunneling process. Comparing (3.26), (3.27), and (3.31), we see that the broken symmetry solution has the lowest energy, but it is not a thermodynamically stable state at finite temperatures. The solution $\varphi = 0$ gives an energy that is very large compared to the energy associated with the kink solution. We see, therefore, that the kinks can be thought of as the elementary excitations above an unstable ground state.

We noted previously that the existence of an instanton for real values of the physical parameters in a theory would lead to the non-Borel summability of a perturbation theory. We might guess and Brézin *et al.*[10-12] have shown, that the existenc of the kinklike solutions lead to the non-Borel sum mability of our double-well model. They find that

$$f(\epsilon) = \sum_{K=0}^{\infty} f_K \epsilon^K\,, \qquad (3.33)$$

where

$$f_K = -\frac{3\sqrt{2}\,K!\,3^K}{\pi 2^{5K/2}}\left[1 + O\left(\frac{1}{K}\right)\right] \qquad (3.34)$$

for large K. It is important to point out that their analysis of the kinklike mode and its relevance to the perturbation theory is considerably more delicate than the corresponding treatment of instantons for metastable systems. The reason is that the kinklike solution is not a periodic solution in the sense we discussed in treating the instantons. Thus, in the particle language we can associate with Eq. (3.11), a particle which leaves the left-hand well will just reach the right-hand well where it stops. It does not return to the left-hand well like a true instanton. In this sense the kink is more like a soliton.

Given the untrustworthiness of a non-Borel summable perturbation theory one wants to find an alternative approach. In the case of a metastable system it was necessary to expand about the tunneling instability—the instanton. In our case it seems reasonable to try the corresponding approach and expand about a kink configuration. This has been carried out by several authors.[30,31] In the Appendix we discuss the technical details. The

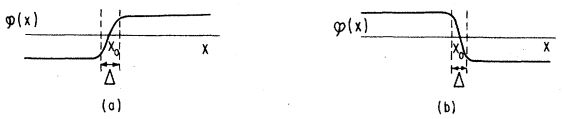

FIG. 3. (a) Kink and (b) antikink field configurations of width $\Delta = 2\sqrt{2}/\kappa$ and position $x = x_0$.

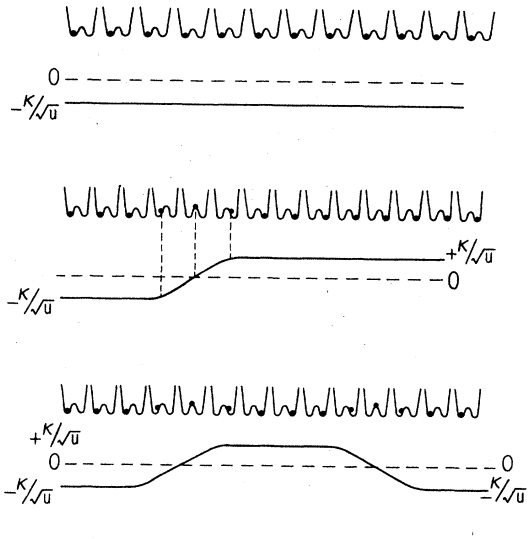

FIG. 4. (a) Classical vacuum, (b) one-kink, and (c) kink-antikink field configurations.

calculation is very similar to that of Langer[5] and Callen and Coleman[7] for the metastable case. A major difference is that in our case, where we deal with a stable system, we find no imaginary contributions to the partition function.

The spirit of these calculations is that one can construct the partition function as a sum of contributions from zero kink, one kink, etc., configurations. Thus we write

$$Z = Z_0 + Z_K + \cdots , \tag{3.35}$$

where Z_K is the contribution from expanding about one kink. We evaluate Z_K in the Appendix taking care to treat the so-called translation mode. If we evaluate Z_K to lowest order in the interaction u we obtain the result

$$Z_K = Z_0 e^{-\beta E_K} V\kappa (32\sqrt{2}/\pi\epsilon)^{1/2} . \tag{3.36}$$

It is clear that if we are to reproduce the thermodynamic limit we must take into account more than just one kink. One kink cannot affect thermodynamic properties. Langer[5] and Callen and Coleman[7] have argued that one can include multikink configuration by ignoring interactions between kinks and essentially just exponentiating Eq. (3.35) to obtain[24]

$$Z = Z_0 \exp(Ve^{-\beta E_K}/a) , \tag{3.37}$$

where

$$a = \kappa^{-1}(32\sqrt{2}/\pi\epsilon)^{-1/2} . \tag{3.38}$$

A more detailed discussion of multikink configurations and their relevance for understanding excited states in quantum mechanics or correlation functions in condensed matter physics is given in Refs. 14 and 15. Their methods for handling multikink configurations appear to us to be extremely cumbersome.

IV. WKB TREATMENT OF PROBLEM

In this section we will carry out an approximate calculation of the partition function Z_φ using the transfer-matrix technique discussed by Scalapino, Sears, and Ferrell[4] and others.[32] Scalapino *et al.* have shown that how one can replace a one-dimensional functional integral by an eigenvalue problem, which in our case essentially amounts to solving a one-particle quantum problem. Briefly, the partition function Z_φ [Eq. (2.3)] can be rewritten as

$$Z_\varphi = \sum_n e^{-V\beta\epsilon_n} , \tag{4.1}$$

where ϵ_n is the energy eigenvalue of the one-dimensional anharmonic Schrödinger equation,

$$\left(-\frac{1}{2\beta^2}\frac{d^2}{dx^2} + V(x) \right) \psi_n(x) = \epsilon_n \psi_n(x) , \tag{4.2}$$

where

$$V(x) = -\tfrac{1}{2}\kappa^2 x^2 + \tfrac{1}{4}ux^4 \tag{4.3}$$

denotes the potential energy of the particle and $\psi_n(x)$ denotes a complete set of normalized eigenstates,

$$\sum_n \psi_n(x)\psi_n^*(x') = \delta(x - x') . \tag{4.4}$$

It is obvious that in the thermodynamic limit when the volume V of the system becomes infinite, the partition function Z_φ is dominated by the lowest eigenstate ϵ_0,

$$Z_\varphi \approx e^{-V\beta\epsilon_0} . \tag{4.5}$$

Our problem then reduces to the evaluation of the ground-state energy eigenvalue ϵ_0 of Eq. (4.2). Notice that the potential energy $V(x)$ has two minima symmetrically located at $\pm\kappa/\sqrt{u}$. At very low temperatures, the particle executes harmonic motion in either of the two potential wells. In the harmonic approximation the doubly degenerate energy spectrum is given by

$$E_n = (n + \tfrac{1}{2})\sqrt{2}\kappa/\beta - \kappa^4/4u , \tag{4.6}$$

where E_n denotes the energy of the nth level. The harmonic approximation is valid only for low-lying energy states. So far we have not considered the quantum-mechanical tunneling through the potential barrier between the two wells which leads to the splitting of each doubly degenerate level. Using the WKB approximation[17] one can evaluate the amount of shift produced in each level due to tunneling. The ground-state energy E_0 (in the harmonic approximation) decreases by an amount

$$t_0 = \frac{\sqrt{2}\kappa}{\pi\beta} \exp\left(-\int_{-x_0}^{x_0} |p|\, dx \right) , \tag{4.7}$$

where

$$\int_{-x_0}^{x_0} |p|\, dx = \int_{-x_0}^{x_0} dx \left[2\beta^2 \left(\frac{ux^4}{4} - \frac{\kappa^2 x^2}{2} - E_0 \right) \right]^{1/2} , \tag{4.8}$$

and $\pm x_0$ are the classical turning points. Without much difficulty, one can show that

$$\int_{-x_0}^{x_0} |p|\, dx = \beta E_K - \ln(16\sqrt{2}e/\epsilon) + O(\epsilon) . \tag{4.9}$$

Therefore, in the presence of tunneling the ground-state energy density of the system is given as

$$\epsilon_0 = E_0 - t_0$$
$$= \left(\frac{\kappa}{\sqrt{2\beta}} - \frac{\kappa^4}{4u} \right) - \frac{\sqrt{2}\kappa}{\pi\beta} \left(\frac{16\sqrt{2}e}{\epsilon} \right)^{1/2} e^{-\beta E_K} . \tag{4.10}$$

After substituting (4.10) into (4.1) we obtain the partition function Z_φ,

$$Z_\varphi = Z_0 \exp(-Ve^{-\beta E_K}/a), \tag{4.11}$$

where

$$Z_0 = \exp(-\beta V E_0) = \exp[-(V\kappa/\sqrt{2} - \beta\kappa^4/4u)] \tag{4.12}$$

is the contribution to the partition function found in perturbation theory to $O(u)$. The parameter a in (4.11) is given by

$$1/a = (\kappa/\pi)(32\sqrt{2}e/\epsilon)^{1/2}. \tag{4.13}$$

On comparing (4.11) with (3.37) we discover that the partition function obtained using the WKB approximation agrees with that of one-kink analysis carried out in Sec. III except for a trivial numerical difference in the value of the parameter a. The ratio

$$\frac{a_{\text{single kink}}}{a_{\text{WKB}}} = \left(\frac{e}{\pi}\right)^{1/2} = 0.93 \tag{4.14}$$

is close to unity.

Scalapino *et al.* have solved the anharmonic Schrödinger equation (4.2) numerically and have obtained the ground-state energy ϵ_0 which agrees fairly well with the E_0 (obtained using the harmonic approximation) at low temperatures. At high temperatures, it deviates from the harmonic approximation due to anharmonic effects and quantum-mechanical tunneling. We will compare our results for the ground-state energy of the system with their exact numerical results in a later section.

V. MULTIKINK APPROACH

Stoll and Schneider[3] and Koehler *et al.*[4] have independently carried out computer simulations for the model given by Eq. (2.1) and have indicated that the existence of the locally ordered regions generate the central peak for small wave numbers q and low temperatures in the dynamic structure factor $S(q, \omega)$. The displacement pattern (shown in Fig. 5) corresponds to a set of large number of kinks sitting side by side and superimposed on it are fluctuations (phonons). This conforms to our picture that in one dimension at finite temperature tunneling between the two wells leads to the formation of multikink configuration. We can mathematically represent the above displacement pattern by the functional transformation

$$\varphi(x) = \Phi(x) + \chi(x), \tag{5.1}$$

where

$$\Phi(x) = \frac{\kappa}{\sqrt{u}} \prod_{i=1}^{N} \tanh\frac{\kappa}{\sqrt{2}}(x - X_i) \tag{5.2}$$

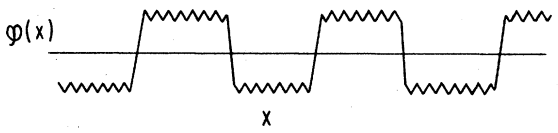

FIG. 5. Schematic of displacement pattern of lattice points as observed in computer simulations at low temperatures.

represents a multikink configuration and $\chi(x)$ corresponds to a set of "residual" phonons. It is essential to treat the multikink field as a product of single kinks if we want to be faithful to the displacement pattern observed in computer simulations. One should realize that we cannot simply insert Eq. (5.1) into Eq. (2.3) since we have not yet given a prescription for determining the kink coordinates X_i. As a first step in giving such a prescription let us introduce an auxiliary quantity:

$$Z_K = \sum_{N=0}^{\infty} \frac{1}{N!} \prod_{i=1}^{N} \int_{-L}^{L} \frac{dX_i}{a} P[X_i]. \tag{5.3}$$

This is just the grand partition function for a set of particles with coordinates X_i and described by a spatial distribution function $P[X_i]$. The parameter a dividing dX_i in (5.3) has dimensions of length and will eventually be identified with the length a given by Eq. (4.12). We now want to associate the particles in Z_K with the kinks in our field theory. This association will arise due to a transformation similar in spirit to the Hubbard-Stratonovich transformation which has been widely used in treating magnetic systems. As a first step in our mapping we multiply and divide Eq. (2.3) by Z_K and write

$$Z_\varphi = \frac{1}{Z_K} \sum_{N=0}^{\infty} \frac{1}{N!} \prod_{i=1}^{N} \int \frac{dX_i}{a} P[X_i] \int \mathfrak{D}\varphi\, e^{-\beta A\{\varphi\}}. \tag{5.4}$$

We then assume that we can take the functional integral over φ inside the X_i integrations. Then we make the transformation (5.1) in (5.4), and rewrite the partition function as

$$Z_\varphi = \frac{1}{Z_K} \sum_{N=0}^{\infty} \frac{1}{N!} \prod_{i=1}^{N} \int \frac{dX_i}{a} P[X_i] \int \mathfrak{D}\chi\, e^{-\beta A\{\Phi+\chi\}}, \tag{5.5}$$

and $A\{\Phi + \chi\}$ will now couple the "phonons" χ and the kinks at positions x_i. We have

$$A\{\Phi + \chi\} = U\{\Phi\} + U\{\chi\} + H_1\{\Phi, \chi\}, \tag{5.6}$$

where $U\{\Phi\}$ is purely a kink contribution, $U\{\chi\}$ a phonon contribution, and

$$H_1\{\Phi,\chi\}=\frac{1}{2}\int dx[2(-\Phi''-\kappa^2\Phi+u\Phi^3)\chi + 3u\Phi^2\chi^2+2u\Phi\chi^3] \quad (5.7)$$

couples the two fields. In this way, we map our original field-theoretic problem into a statistical-mechanical problem of a gas of kinks and interacting phonons.

Let us begin with a discussion of the kink contribution. In order to gain some feeling for the form of $U\{\Phi\}$ let us first look at the quantity $\Phi^2(x)$ which appears in $U\{\Phi\}$. This can be written

$$\Phi^2(x)=\frac{\kappa^2}{u}\prod_{i=1}^{N}\tanh^2\frac{\kappa}{\sqrt{2}}(x-X_i) =\frac{\kappa^2}{u}\prod_{i=1}^{N}[1+C_i(x)], \quad (5.8)$$

where $C_i(x)=-\cosh^{-2}(\kappa/\sqrt{2})(x-X_i)$. This can be rewritten as

$$\Phi^2(x)=\frac{\kappa^2}{u}\left(1+\sum_{i=1}^{N}C_i(x)+\frac{1}{2}\sum_{i\neq j=1}^{N}C_i(x)C_j(x)+\cdots\right), \quad (5.9)$$

where additional terms involve sums over terms involving three and higher distinct number of particles. If the density of kinks is small, then each of these terms will contribute, on averaging, a factor of the density of kinks for each distinct sum in a term. Thus, for example, the average of the term $\sum_{i\neq j=1}^{N}C_i(x)C_j(x)$ will be second order in the kink density. Using these ideas we can rewrite the kink Hamiltonian in the form

$$U\{\Phi\}=NE_K+U_1\{\Phi\}-\kappa^4V/4u, \quad (5.10)$$

where E_K is just the kink energy given by Eq. (3.32) and

$$U_1\{\Phi\}=\sum_{i\neq j=1}^{N}U_2(X_i-X_j)+\sum_{i\neq j\neq k=1}^{N}U_3(X_i,X_j,X_k)+\cdots, \quad (5.11)$$

where the dots represent higher-order interactions, is the interaction between kinks. We calculate directly that the pair interaction between kinks is

$$U_2(x)=E_K\,\mathrm{csch}^2\frac{\kappa x}{\sqrt{2}}\left(1+5\coth^2\frac{\kappa x}{\sqrt{2}}-\frac{15\kappa x}{2\sqrt{2}}\coth^3\frac{\kappa x}{\sqrt{2}} -\frac{15}{2}\coth^4\frac{\kappa x}{\sqrt{2}}+\frac{15\kappa x}{2\sqrt{2}}\coth^5\frac{\kappa x}{\sqrt{2}}\right). \quad (5.12)$$

We note that the two-body potential falls off exponentially for large distances and is attractive (see Fig. 6). At large distances our result for the kink-kink interaction agrees with that obtained by Rajaraman[33] using quite different techniques. The three-body potential can be shown to be short ranged, e.g.,

$$\lim_{k,q\to0}U_3(k,q)=\lim_{k,q\to0}\int d(x_i-x_j)d(x_i-x_l)\times e^{ik(x_i-x_j)}e^{iq(x_i-x_l)}U(X_i,X_j,X_l) =-4\sqrt{2}\kappa/u=-6E_K/\kappa^2. \quad (5.13)$$

We believe that the correct physical picture of our system is that of a low density kink gas at low temperatures. We see, however, that the interaction $U_1\{\Phi\}$ between kinks is attractive. This means, of course, that our system is unstable at low temperatures to the formation of kink-antikink bound pairs and, at low enough temperatures, because of the many-body interactions, we expect this system to collapse to a large number of kinks at a point. This collapse is an intolerable feature and does not occur in the molecular dynamics simulations. We can restabilize our kink system via a judicious choice for the probability distribution for the "vacuum" kinks $P[X_i]$. We choose $P[X_i]$ so that the attractive interactions between kinks $U_1\{\Phi\}$ is cancelled. We write therefore

$$P[X_i]=e^{\beta U_i\{\Phi\}}, \quad (5.14)$$

then

$$Z_K=\sum_{N=0}^{\infty}\frac{1}{N!}\prod_{i=1}^{N}\int\frac{dX_i}{a}e^{\beta U_1\{\Phi\}} \quad (5.15)$$

represents the grand partition function for a set of kinks interacting via repulsive interactions. Combining Eqs. (5.5), (5.6), (5.10), and (5.14) the partition function can then be written as

$$Z_\varphi=\frac{e^{E_V}}{Z_K}\sum_{N=0}^{\infty}\frac{e^{-\beta E_K N}}{N!}\prod_{i=1}^{N}\int\frac{dX_i}{a}\times\int\mathfrak{D}\chi\exp[-\beta(U\{\chi\}+H_1\{\Phi,\chi\})]. \quad (5.16)$$

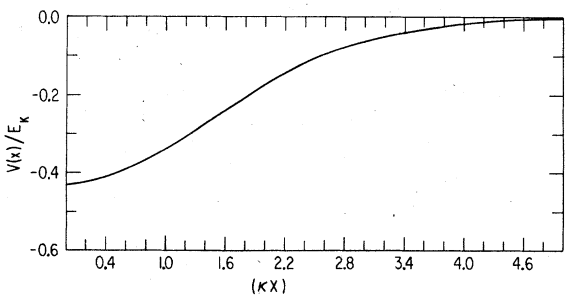

FIG. 6. Interaction potential $V(x)$ vs x between a kink and an antikink. For small x, $V(x)\approx(-\frac{3}{7}+\frac{5}{96}\kappa^2x^2)E_K$. Whereas for large distances $V(x)=-6E_K\exp(-\sqrt{2}\kappa x)$.

The kinks in the numerator interact with each other only through interactions with the phonons. Note that we now have a term $\exp(-\beta N E_K)$ in the weight factor. We see that $-E_K$ is essentially the chemical potential associated with kink creation and, as we will verify, the kink density at low temperatures will be proportional to $\exp(-\beta E_K)$.

Let us now focus on the part of the Hamiltonian coupling Φ and χ defined by Eq. (5.7). Let us analyze H_1 using the result (5.9) for $\Phi^2(x)$. After some elementary algebra and noticing a cancellation that follows from the stationarity of $V[\varphi]$ in the presence of one kink,

$$H_1\{\Phi,\chi\}=\frac{3\kappa^2}{2}\int dx\,\chi^2(x)+u\int dx\,\Phi(x)\chi^3(x) + 3\kappa^2\int dx\,dx'\,n(x)\chi^2(x') \times\left(\frac{-1}{\cosh^2(\kappa/\sqrt{2})(x-x')}\right)+\cdots, \quad (5.17)$$

where the dots represent terms involving two distinct kinks and

$$n(x)=\sum_{i=1}^{N}\delta(x-X_i) \quad (5.18)$$

is the kink density "operator." We see that the first term really does not couple the kinks to phonons and should be lumped with $U\{\chi\}$ as the basic phonon Hamiltonian. The second term can be treated as a perturbation in u and the third- and higher-order terms are small when the kink density is small. We can therefore write the effective "Hamiltonian" after our transformations as

$$U\{\chi\}+H_1\{\Phi,\chi\}=F\{\chi\}+H_I\{\chi,\Phi\}, \quad (5.19)$$

where

$$F\{\chi\}=\frac{1}{2}\int dx\left[\left(\frac{\partial\chi}{\partial x}\right)^2+2\kappa^2\chi^2+\frac{u\chi^4}{2}\right], \quad (5.20)$$

and

$$H_I\{\chi,\Phi\}=\frac{1}{2}\int dx\left\{2\chi(x)[-\Phi''(x)+u\Phi^3(x)-\kappa^2\Phi(x)] + 2u\Phi\chi^3+3u\left(\Phi^2-\frac{\kappa^2}{u}\right)\chi^2(x)\right\}. \quad (5.21)$$

We see then that H_I can be treated as a perturbation if u is small and the kink density is small. We also note that $F\{\chi\}$ represents the Hamiltonian for a *single-well* oscillator. There are no problems in using perturbation theory to treat the χ phonons.[10]

Now we can calculate any physical quantity of interest. For example, the average of any variable $A(\varphi)$ is given as

$$\langle A(\varphi)\rangle=\frac{1}{Z}\sum_{N=0}^{\infty}\frac{1}{N!}\prod_{i=1}^{N}\int\frac{dX_i}{a}\,e^{-\beta N E_K} \times\int\mathfrak{D}\chi\exp(-\beta[F_0\{\chi\}+\lambda H_c\{\Phi,\chi\}])A\{\Phi+\chi\}, \quad (5.22)$$

where

$$Z=\sum_{N=0}^{\infty}\frac{1}{N!}\prod_{i=1}^{N}\int\frac{dX_i}{a}\,e^{-\beta N E_K} \times\int\mathfrak{D}\chi\exp(-\beta[F_0\{\chi\}+\lambda H_c\{\Phi,\chi\}]), \quad (5.23)$$

and we have included the quartic part of $F[\chi]$ in H_c:

$$F_0\{\chi\}=\frac{1}{2}\int dx\left[\left(\frac{\partial\chi}{\partial x}\right)^2+2\kappa^2\chi^2\right], \qquad H_c\{\Phi,\chi\}=H_I\{\Phi,\chi\}+\int dx\,\frac{u}{4}\chi^4(x). \quad (5.24)$$

We have introduced λ in (5.22) so as to keep track of various terms in the perturbation-series expansion in H_c.

VI. THERMODYNAMIC PROPERTIES

In this section we will evaluate the density of the kinks and other thermodynamic properties of our kink-phonon system. The average density of the kinks is written as

$$n(\lambda)=\frac{1}{V}\frac{\partial}{\partial\alpha}G(\alpha,\lambda), \quad (6.1)$$

where

$$G(\alpha,\lambda)=\ln\sum_{N=0}^{\infty}\frac{1}{N!}\prod_{i=1}^{N}\int\frac{dX_i}{a}\,e^{N\alpha} \times\int\mathfrak{D}\chi\exp(-\beta F_0\{\chi\}-\beta\lambda H_c\{\Phi,\chi\}), \quad (6.2)$$

and $a=-\beta E_K$. We have calculated $G(\alpha,\lambda)$ to the second order in λ and found it to be well behaved. We discuss here only our results to the first order in λ,

$$G(\alpha,\lambda)=-V\kappa[1/\sqrt{2}-\xi+\lambda\eta(\epsilon)], \quad (6.3)$$

where

$$\xi=n_0/\kappa=e^{-\beta E_K}/\kappa a \quad (6.4)$$

is the dimensionless free kink density and $\eta(\epsilon)$ is the first-order correction given by

$$\eta(\epsilon)=[(3/4\sqrt{2})(e^{-2\sqrt{2}\epsilon}-1)+\tfrac{3}{32}\epsilon]. \quad (6.5)$$

Remember $\epsilon=uk_BT/\kappa^3$ is the dimensionless parameter introduced in Sec. II. Using (4.11), (6.3), and (6.1) we obtain the average density of the kinks

$n(\lambda)$ in the presence of the interaction,

$$n(\lambda) = (1/\Delta)\exp[-\beta E_K(T)]\,, \tag{6.6}$$

where $\Delta = 2\sqrt{2}/\kappa$ is the width of a kink and

$$E_K(T) = E_K\left[1 - \frac{3}{2\sqrt{2}}\,\epsilon \ln\left(\frac{(256\sqrt{2}e)^{1/2}}{\pi}\right) + \frac{3}{4\sqrt{2}}\,\epsilon\ln\epsilon - \frac{9\lambda\epsilon}{4\sqrt{2}}\,e^{-2\sqrt{2}\xi}\right] \tag{6.7}$$

is temperature-dependent kink energy. By setting $\lambda = 0$, we recover free kink density

$$n(\lambda = 0) = n_0 = [(32\sqrt{2}e)^{1/2}/\pi\sqrt{\epsilon}\,]\,e^{-\beta E_K}\,. \tag{6.8}$$

We plot the free and interacting kink densities in Fig. 7. We observe that as soon as we turn on the interaction, the average density of the kinks increases.

We also plot the temperature-dependent kink energy $E_K(T)$ vs ϵ in Fig. 8 for the free ($\lambda = 0$) and interacting ($\lambda = 1$) cases. In the presence of interactions, the energy required to create a kink decreases. Also we observe that the kink energy E_K decreases with the increase of temperature. Koehler *et al.*[4] have determined the temperature-dependent kink energy $E_K(T)$ in two ways. They have evaluated $E_K(T)$ from the static structure factor using the transfer-matrix technique and obtained approximately that

$$E_K(T) = E_K(1 - 3\sqrt{2}\epsilon)\,, \tag{6.9}$$

which we also plot in Fig. 8. They have also carried out molecular dynamics simulations on the associated lattice model. One can extract rough estimates for the kink density from these lattice calculations. For $\lambda = 1$ and at low temperatures, our analysis predicts higher kink density compared to the one obtained using transfer-matrix technique by Koehler *et al.* But their average density of the kinks by this method is much lower than what is observed in computer simulations. So our result for the average kink density is in better agreement with computer simulations than the transfer-matrix result given by Eq. (6.9).

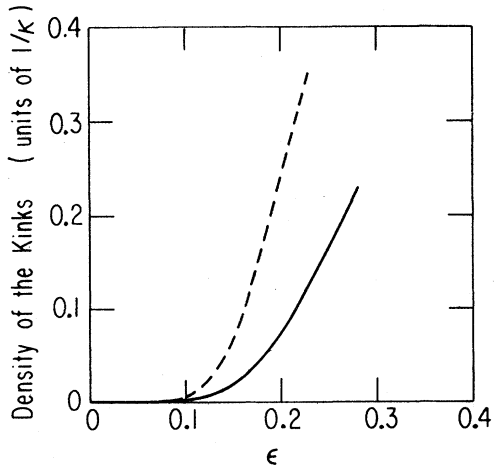

FIG. 7. Density of the kinks $n(\lambda)$ vs ϵ for $\lambda = 0$ (solid line) and $\lambda = 1$ (dashed line).

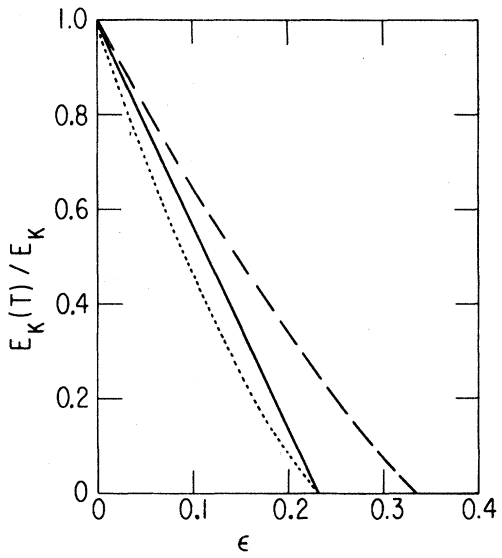

FIG. 8. Temperature-dependent kink energy $E_K(T$ vs ϵ for $\lambda = 0$ (dashed line) and $\lambda = 1$ (dotted line). The solid line is due to Koehler *et al.*

Next we evaluate the energy density of the kink-phonon system. Using (5.22) we write the average energy density as

$$E/V = [\tfrac{1}{4}u\langle\langle(\Phi+\chi)^4\rangle - \tfrac{1}{2}\kappa^2\langle\langle(\Phi+\chi)^2\rangle + \tfrac{1}{2}\langle\langle(\Phi'+\chi')^2\rangle\rangle]\,. \tag{6.10}$$

After a little algebra, one can evaluate the energy density to the first order in λ and n as

$$\frac{Eu}{V\kappa^4} = \left\{\left[-\frac{1}{4} + \left(\frac{1}{\sqrt{2}} + \frac{3\epsilon}{8}\right)\epsilon + \left(\frac{2\sqrt{2}}{3} - \frac{3}{2}\,\epsilon\right)\xi\right] + \lambda\left[-\frac{1}{2}\,\epsilon^2 + \xi\left(\frac{7}{3} - 3\epsilon + \frac{5}{4}\,\epsilon^2\right)\right]\right\}. \tag{6.11}$$

In the absence of interaction ($\lambda = 0$), and at low temperatures, the energy density of the phonon-kink system is given as

$$\frac{E}{V} = -\frac{\kappa^4}{4u} + \frac{1}{\sqrt{2}}\,\kappa k_B T + nE_K\,. \tag{6.12}$$

The first term in (6.12) corresponds to vacuum energy, the second and third terms are the phonon and kink energy densities, respectively. At $T = 0$,

$$E = -\kappa^4 V/4u = E_{\text{vac}}\,. \tag{6.13}$$

This result is no surprise to us as at zero tem-

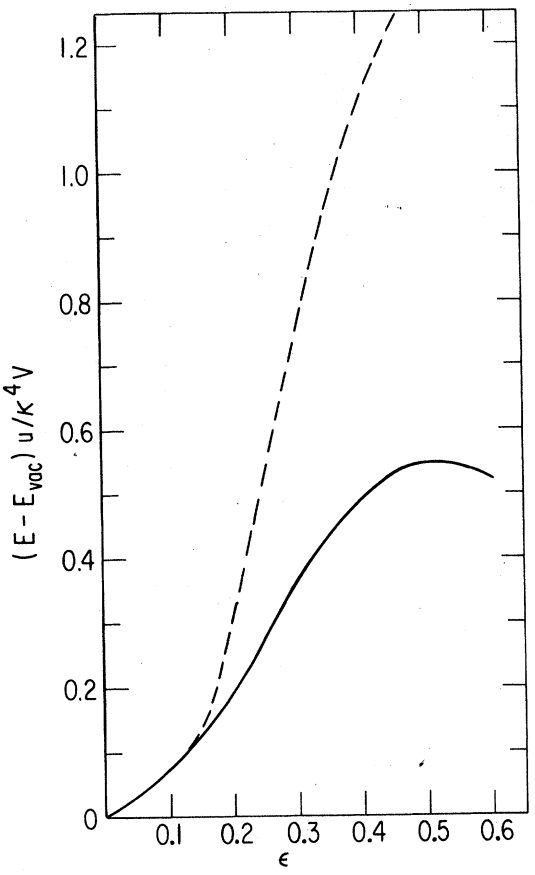

FIG. 9. Energy of the kink-phonon system vs ϵ for $\lambda=0$ (solid line) and $\lambda=1$ (dashed line).

perature all atoms sit in either of the two wells and then $\varphi_c=\pm\kappa/\sqrt{u}$ which on substituting in (2.1) gives (6.13). In Fig. 9 we plot $(E-E_{vac})u/V\kappa^4$ vs ϵ. As soon as we turn on the interaction, the energy density of the kink-phonon system increases considerably.

Now the specific heat of the kink-phonon system can be readily obtained from the energy density,

$$\frac{C}{\kappa V}=k_B\left\{\left[\left(\frac{1}{\sqrt{2}}+\frac{3}{4}\epsilon\right)+\xi\left(\frac{8}{9\epsilon^2}-\frac{3}{2}-\frac{\sqrt{2}}{\epsilon}\right)\right]+\lambda\left[-\epsilon+\frac{2\sqrt{2}}{3\epsilon^2}\,\xi\left(\frac{7}{3}-3\epsilon+\frac{5}{4}\epsilon^2\right)+\xi\left(-3+\frac{5}{2}\epsilon\right)\right]\right\}. \tag{6.14}$$

At low temperatures and in the absence of interaction, the specific heat is given by

$$C/\kappa V=k_B(1/\sqrt{2}+8\xi/9\epsilon^2). \tag{6.15}$$

The first term in (6.15) is the contribution to the specific heat due to a classical gas of phonons and the second term corresponds to the specific heat of free kinks. At low temperatures, the specific heat due to kinks is in good agreement with that of one-dimensional Ising model suggesting thereby that at low temperatures, the system of atoms behaves like Ising spins. One can understand this situation as follows; at low temperatures, due to quantum-mechanical tunneling, an individual atom randomly tunnels through to the other well which is equivalent to flipping a spin in a system of aligned spins.

We plot $C/\kappa Vk_B$ vs ϵ in Fig. 10. We also observe a maxima in the specific heat as reported by other authors.[20,34] In the presence of interaction, the specific heat increases compared to that of free kink-phonon system.

VII. STATIC-CORRELATION FUNCTION

A. Basic development

The basic quantity giving us information about the equilibrium structure in our system is the static structure factor

$$S(k)=\int_{-\infty}^{\infty}d(x-x')\,e^{-ik(x-x')}\langle\delta\varphi(x)\delta\varphi(x')\rangle. \tag{7.1}$$

After we make our functional transformation $\varphi=\Phi+\chi$ the structure factor reduces to a sum of three pieces,

$$S(k)=S_K(k)+S_p(k)+2S_c(k), \tag{7.2}$$

where

$$S_K(k)=\int_{-\infty}^{\infty}d(x-x')\,e^{-ik(x-x')}\langle\delta\Phi(x)\delta\Phi(x')\rangle \tag{7.3}$$

is the kink-kink structure factor,

$$S_p(k)=\int_{-\infty}^{\infty}d(x-x')\,e^{-ik(x-x')}\langle\delta\chi(x)\delta\chi(x')\rangle \tag{7.4}$$

is the phonon-phonon structure factor, and

$$S_c(k)=\int_{-\infty}^{\infty}d(x-x')\,e^{-ik(x-x')}\langle\delta\chi(x)\delta\Phi(x')\rangle \tag{7.5}$$

is the "cross-correlation" function correlating kink and phonon fields. We can now develop a perturbation series expansion for these correlation functions in terms of the parameter λ.

B. Kink-kink correlation function

We can easily evaluate $S_K(x-x')$ to zeroth order in λ to obtain

$$S_K^0(x-x')=\frac{\kappa^2}{u}\exp\left(-2n_0(x-x')\coth\frac{\kappa}{\sqrt{2}}(x-x')\right). \tag{7.6}$$

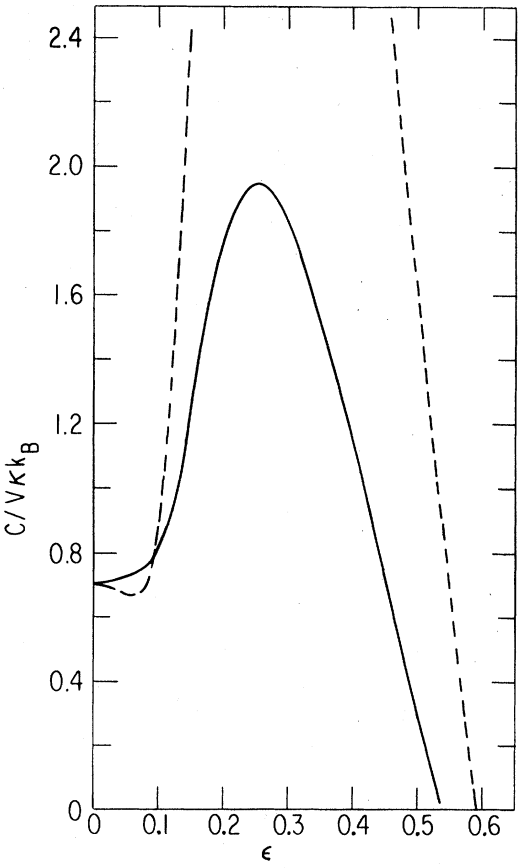

FIG. 10. Specific heat of the kink-phonon system vs ϵ for $\lambda=0$ (straight line) and $\lambda=1$ (dashed line).

We see then, for large separations, the correlation function decays as

$$S_K^0(x-x') \xrightarrow[|x-x'|\to\infty]{} \frac{\kappa^2}{u} e^{-2n_0|x-x'|}, \tag{7.7}$$

and we can identify the correlation length $(2n_0)^{-1}$. As $T\to 0$ and $n_0\to 0$, this correlation length becomes infinite announcing the zero-temperature phase transition in this system.

We have not been able to compute $S_K^0(k)$ analytically. However, the approximate form

$$\tilde{S}_K^0(k)=\frac{\kappa^2}{u}\left(\frac{4n_0}{4n_0^2+k^2}\right)\exp(-2\sqrt{2}n_0/\kappa) \tag{7.8}$$

follows from the interpolation between the large and small $|x-x'|$ limits:

$$\tilde{S}_K^0(x-x')\simeq\frac{\kappa^2}{u}\exp(-2\sqrt{2}n_0/\kappa)\exp(-2n_0|x-x'|). \tag{7.9}$$

As we see from Fig. 11, $\tilde{S}_K^0(k)$ compares favorably with $S_K^0(k)$, evaluated numerically, over a wide range of wave numbers. It is easy to show that

$$S_K^0(k=0)=\frac{2\sqrt{2}\kappa}{u}\left(\frac{1}{2\sqrt{2}\xi}-\frac{\pi^2}{4\epsilon}+O(\xi)\right), \tag{7.10}$$

where $\xi=n_0/k$. The main point is that the kink-structure factor is very sharply peaked about $k=0$ for low temperatures.

We can now proceed to investigate the corrections to $S_K^0(k)$ using λ as an expansion parameter. It is easy to show that the first-order correction to S_K is given by

$$S_K^{(1)}(x-x')=-\frac{3u\lambda}{4\sqrt{2}\kappa}\int dy[\langle\Phi^2(y)\Phi(x)\Phi(x')\rangle_0 - \langle\Phi^2(y)\rangle_0 S_K^0(x-x')], \tag{7.11}$$

where we have used

$$\langle\chi^2(y)\rangle_0=1/2\sqrt{2}\beta\kappa. \tag{7.12}$$

A key point here is to remember that the fields Φ are not Gaussian for $\lambda=0$. We are so conditioned to think in terms of Gaussian variables that it is

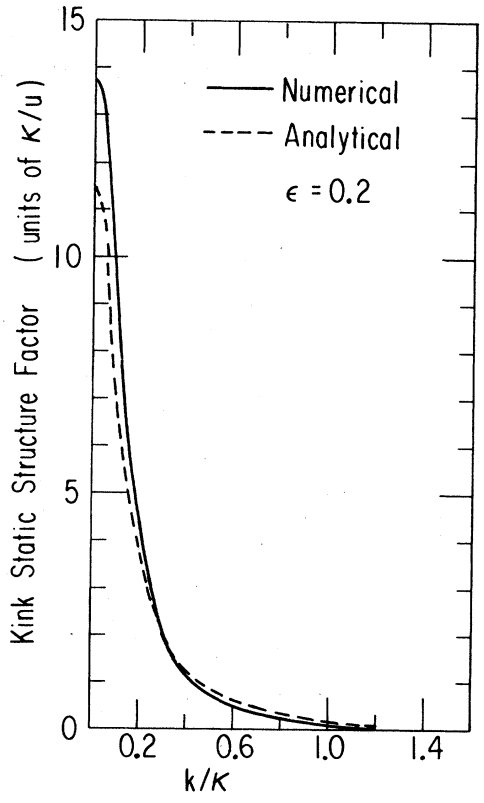

FIG. 11. Comparison of the numerical (solid line) and analytical (dashed line) result of the kink static structure factor.

tempting to evaluate $S_K^{(1)}$ in the approximation where we replace the four-point Φ correlation function by its disconnected pieces. This standard Dyson equation approach leads[5] to the result

$$S_K^{-1}(k) = S_K^{0-1}(k) + 3u\lambda/2\sqrt{2}\kappa\,, \tag{7.13}$$

with the consequence that as $k \to 0$ and $T \to 0$, S_K is finite! As we shall see this reasoning is faulty. A direct analysis of (7.11) leads to

$$S_K^{(1)}(x-x') = -\frac{3\kappa\lambda}{2\sqrt{2}}\, S_K^0(x-x')e^{-2\sqrt{2}\xi} \times \int dy\,\{\exp[-n_0 k_0(y,x,x')] - 1\}\,, \tag{7.14}$$

where

$$K_0(y,x,x') = \int dz\, \frac{\tanh(\kappa/\sqrt{2})(x-z)\tanh(\kappa/\sqrt{2})(x'-z) - 1}{\cosh^2(\kappa/\sqrt{2})(y-z)}\,. \tag{7.15}$$

We are interested in evaluating $S^{(1)}$ to lowest order in n_0. If we expand to first order in n_0 in (7.14) and then carry out the y integration we obtain

$$S_K^{(1)}(x-x') = \frac{3\lambda n_0}{2}\frac{\partial}{\partial n_0} S_K^0(x-x')\,, \tag{7.16}$$

or

$$S_K(x-x') = \left[1 + \tfrac{3}{2}\lambda n_0 \frac{\partial}{\partial n_0} + O(\lambda^2, \lambda n_0^2)\right] S_K^0(x-x') = \left[\exp\left(\tfrac{3}{2}\lambda n_0 \frac{\partial}{\partial n_0}\right) + O(\lambda^2, \lambda n_0^2)\right] S_K^0(x-x')\,. \tag{7.17}$$

If we use Eq. (7.6) and make the change of variable to $y = \ln(n_0/\kappa)$, then [with $f(x) = 2\kappa x \coth(\kappa x/\sqrt{2})$]

$$S_K(x-x') = \exp\left(\frac{3}{2}\lambda\frac{\partial}{\partial y}\right)\frac{\kappa^2}{u}\exp[e^y f(x-x')] = \frac{\kappa^2}{u}\exp[e^{(y+3\lambda/2)} f(x-x')]\,. \tag{7.18}$$

We see from Eq. (6.6) that

$$n = n_0 e^{3\lambda/2}[1 + O(\lambda, n_0)]\,, \tag{7.19}$$

and

$$S_K(x-x') = \frac{\kappa^2}{u}\exp[-2nx\coth(x\kappa/\sqrt{2})] \times [1 + O(\lambda^2, \lambda n_0^2)]\,, \tag{7.20}$$

so that we simply replace $n_0 \to n$ in first order in λ. Then, for example,

$$S_K(k=0) = \frac{2\sqrt{2}\kappa}{\sqrt{u}}\left(\frac{1}{2\sqrt{2}n/\kappa} - \frac{\pi^2}{4\epsilon} + O(\lambda^2, \lambda n_0^2)\right), \tag{7.21}$$

and $S_K(k=0)$ diverges as $T \to 0$ as $1/n$. This contradicts the results of the "disconnected" approximation and should be sufficient to contain our desire to apply a Dyson equation analysis to our problem. While resummations are required, they must be developed in a manner different from the conventional self-energy resummation. Again we can approximate $S_K(k)$ with Eq. (7.8) with $n_0 \to n$ and write

$$\tilde{S}_K(k) = \frac{\kappa^2}{u}\, e^{-2\sqrt{2}n/\kappa}\left(\frac{4n}{4n^2 + k^2}\right). \tag{7.22}$$

We plot the total static structure factor for $\lambda = 0$ and $\lambda = 1$ in Fig. 13. We discover that as soon as we turn on the interaction, the peak of $S_K(k)$ decreases in height and becomes broad as expected.

C. Phonon-phonon correlation function

Now we evaluate the phonon static structure factor. To second order in λ^2 we have

$$S_\rho(k) = \int_{-\infty}^{\infty} d(x-x')\, e^{-ik(x-x')}\langle\delta\chi(x)\delta\chi(x')\rangle = S_\rho^0(k) + \lambda S_\rho^{(1)}(k) + \lambda^2 S_\rho^{(2)}(k) + \cdots\,, \tag{7.23}$$

where $S_\rho^0(k)$ is the free-phonon static structure factor and can be easily shown to be equal to

$$S_\rho^0(k) = \int_{-\infty}^{\infty} d(x-x')\, e^{-ik(x-x')}\langle\delta\chi(x)\delta\chi(x')\rangle_0 = \frac{1}{\beta(k^2 + 2\kappa^2)}\,. \tag{7.24}$$

The first-order term can be written as

$$S_\rho^{(1)}(k) = -\beta\int_{-\infty}^{\infty} d(x-x')\, e^{-ik(x-x')} \times \int dy\langle\delta H_I(y)\delta\chi(x)\delta\chi(x')\rangle_0 = S_\rho^0(k)\Sigma_\rho(k)S_\rho^0(k)\,, \tag{7.25}$$

where the first-order phonon self-energy is given by

$$\Sigma_\rho(k) = -\lambda[\tfrac{3}{2}\kappa^2\beta(e^{-2\sqrt{2}\xi} - 1) + 3u\beta S_\rho^0(0)] \tag{7.26}$$

and

$$S_\rho^0(0) = \langle\chi^2(x)\rangle_0 = 1/2\sqrt{2}\beta\kappa\,. \tag{7.27}$$

A careful analysis of the second-order static structure factor $S_\rho^{(2)}(k)$ suggests that apart from the usual phonon self-energy diagrams, it contains a diagram [Fig. 12(a)] which requires a special attention. The dotted line in Fig. 12(a) represents

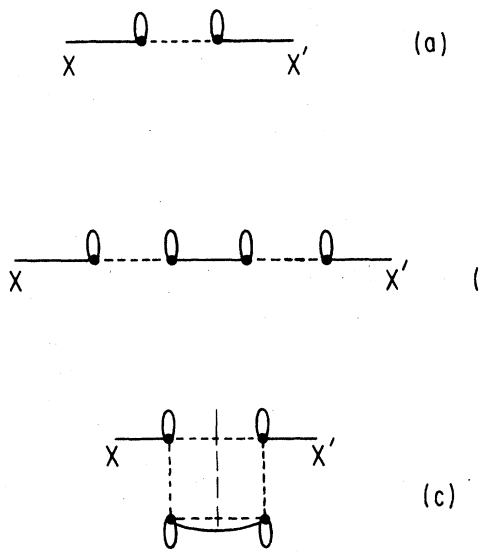

FIG. 12. (a) Second-order graph which does not contribute to the self-energy. (b) Fourth-order graph obtained by cutting along the vertical line a fourth-order graph (c) appearing in the perturbation series.

kink-kink correlation function and the solid line corresponds to phonon-phonon correlation function. The Fourier transform of the above diagram is proportional to the kink static structure factor which goes as the inverse of the kink density for $k=0$. At very low temperatures, it is the dominant contribution to phonon static structure factor. If one simply includes the contribution of this term in the phonon self-energy, one obtains a phonon static structure factor which goes negative for $k=0$ at low temperatures. This is quite unphysical! It appears that one should not regard this diagram as a phonon self-energy diagram. If indeed Fig. 12(a) were to be interpreted as contributing to the phonon self-energy a fourth-order diagram of the form given in Fig. 12(b) should appear. Such a graph would occur if we were to disconnect the fourth-order diagram shown in Fig. 12(c). We learned earlier in treating the kink static-structure factor that we cannot treat the kink field $\Phi(x)$ as a Gaussian variable. Consequently we should not disconnect Fig. 12(c) to obtain Fig. 12(b) and the contribution in Fig. 12(a) should not be treated as a self-energy correction. So to the second order in λ, we keep track of the above diagram and resume the rest of diagrams to write the phonon-correlation function in the form

$$S_\rho(k)=S_\rho^0(k)+S_\rho^0(k)\Sigma_\rho(k)S_\rho(k)+S_\rho^0(k)\Sigma_K(k)S_\rho^0(k)\,, \tag{7.28}$$

where the phonon self-energy $\Sigma_\rho(k)$ is given by Eq. (7.26)

$$\Sigma_\rho(k)=-\lambda\left[\tfrac{3}{2}\kappa^2\beta(e^{-2\sqrt{2}\xi}-1)+3u\beta S_\rho^0(0)\right]\,, \tag{7.29}$$

and

$$\Sigma_K(k)=9\lambda^2\beta^2u^2[S_\rho^0(0)]^2S_K^0(k) \tag{7.30}$$

is the second-order contribution from the graph in Fig. 12(a).

We can then solve for $S_\rho(k)$ and substitute Eq. (7.24) for $S_\rho^0(k)$ to obtain

$$S_\rho(k)=\frac{1+\Sigma_K(k)S_\rho^0(k)}{\beta(k^2+2\kappa^2-\Sigma_\rho(-k)/\beta)}=\frac{1+\Sigma_K(k)S_\rho^0(k)}{\beta(k^2+\kappa_\rho^2)}\,, \tag{7.31}$$

where

$$\kappa_\rho^2=2\kappa^2+\lambda\left[\tfrac{3}{2}\kappa^2(e^{-2\sqrt{2}\xi}-1)+3uS_\rho^0(0)\right]. \tag{7.32}$$

For $k\neq0$, as $T\to0$ we recover the free-phonon static structure factor,

$$\lim_{T\to0}S_\rho(k)=\frac{1}{\beta(k^2+2\kappa^2)}=S_\rho^0(k)\,. \tag{7.33}$$

At $k=0$, the phonon static structure factor is given by

$$S_\rho(0)=[1+\Sigma_K(0)S_\rho^0(0)]/\beta\kappa_\rho^2\,. \tag{7.34}$$

If we restrict our analysis to the first order in λ, we find that

$$\lim_{T\to0}\beta S_\rho(0)=\frac{1}{2\kappa^2}+O(\lambda^2) \tag{7.35}$$

is finite. Whereas if we include $O(\lambda^2)$ terms in our analysis, we discover that

$$\lim_{T\to0}\beta S_\rho(0)=\frac{9\lambda^2\epsilon}{8\xi\kappa^2}\to\infty\,. \tag{7.36}$$

This clearly emphasizes the importance of the second-order graph shown in Fig. 12(a). We have also convinced ourselves that the product of such graphs does not occur in higher orders.

D. Cross-correlation function

Next we evaluate the cross correlation function. To the second order in λ, one finds that

$$\begin{aligned}S_c(x-x')&=\langle\chi(x)\Phi(x')\rangle\\&=-\beta\lambda\int dy\,\langle\delta H_I(y)\chi(x)\Phi(x')\rangle_0\\&\quad+\beta^2\lambda^2\int dy\int dy'\langle\delta H_I(y)\delta H_I(y')\\&\qquad\times\chi(x)\Phi(x')\rangle_0\,.\end{aligned} \tag{7.37}$$

The zero-order term vanishes due to the fact that the zero-order phonon and kink Hamiltonians are even their variables. Rewriting Eq. (7.37) explicitly to the first order in λ,

$$S_c(x-x') = -\beta\lambda u \int dy \langle \chi^3(y)\chi(x)\rangle_0 \langle \Phi(y)\Phi(x')\rangle_0 - \beta\lambda \int dy \langle \chi(y)\chi(x)\rangle_0 \langle [-\Phi'(y) - \kappa^2\Phi(y) + u\Phi^3(y)]\Phi(x')\rangle_0$$
$$+ \beta^2\lambda^2 \int dy \int dy \langle \delta H_I(y)\delta H_I(y')\chi(x)\Phi(x')\rangle_0$$
$$= -3\beta\lambda u \int dy\, S_\rho^0(x-y)S_\rho^0(0)S_K^0(y-x') - \beta\lambda \int dy\, S_\rho^0(y-x)(n_0^2-\kappa^2)S_K^0(y-x')$$
$$-\beta\lambda u \int dy\, S_\rho^0(y-x)\langle \Phi^3(y)\Phi(x')\rangle_0 + \beta^2\lambda^2 \int dy \int dy' \langle \delta H_I(y)\delta H_I(y')\chi(x)\Phi(x')\rangle_0 . \quad (7.38)$$

It can be shown that

$$\langle \Phi^3(y)\Phi(x')\rangle_0 = (\kappa^2/u)S_K^0(y-x')e^{-n_0 Q(y-x')}, \quad (7.39)$$

where the function $Q(x)$ is given by

$$Q(x) = \frac{2\sqrt{2}}{\kappa \sinh^2(\kappa x/\sqrt{2})}\left(\frac{\kappa x}{\sqrt{2}\tanh(\kappa x/\sqrt{2})} - \frac{\tanh(\kappa x/\sqrt{2}) + \operatorname{sech}^2(\kappa x/\sqrt{2})}{1+\tanh(\kappa x/\sqrt{2})}\right). \quad (7.40)$$

$Q(x)$ is finite as $x \to 0$ and is given as

$$Q(0) = 2\sqrt{2}/3\kappa , \quad (7.41)$$

and leads to the result

$$\langle \Phi^4(x)\rangle_0 = (\kappa^4/u^2)e^{-8\sqrt{2}n_0/\kappa}. \quad (7.42)$$

At large distance, $Q(x)$ falls off exponentially,

$$Q(x) \approx 8xe^{-\sqrt{2}\kappa x}, \quad (7.43)$$

which goes to zero as $x \to \infty$. So for large distances, we can approximate

$$\langle \Phi^3(y)\Phi(x')\rangle_0 \approx (\kappa^2/u)S_K^0(y-x'), \quad (7.44)$$

which has the same functional form as that of the two-kink correlation function. Substitute (7.55) in (7.49) and obtain

$$S_c(x-x') = -3\beta\lambda u \int dy\, S_\rho^0(y-x)S_\rho^0(0)S_K^0(y-x')$$
$$-\beta\lambda n_0^2 \int dy\, S_\rho^0(y-x)S_K^0(y-x')$$
$$+\beta^2\lambda^2 \int dy \int dy' \langle \delta H_I(y)\delta H_I(y')\chi(x)\Phi(x')\rangle_0 . \quad (7.45)$$

If we analyze the second-order terms, we find that there are some terms which renormalize the kink correlation function appearing in (7.45). We can then rewrite the cross correlation function as

$$S_c(x-x') = -3\beta\lambda u \int dy\, S_\rho^0(y-x)S_\rho^0(0)S_K(y-x')$$
$$+ O(n_0^2, \lambda^2). \quad (7.46)$$

We next Fourier transform the space coordinates to obtain the cross static structure factor to the first order in λ,

$$S_c(k) = -3\beta\lambda u S_\rho^0(k)S_\rho^0(0)S_K(k)$$
$$+ O(n_0^2, \lambda^2). \quad (7.47)$$

At $k=0$, the cross static structure factor grows exponentially as temperature is lowered towards the critical temperature $T=0$.

Adding (7.22), (7.31), and (7.47), we obtain the total static structure factor $S_T(k)$. We plot $S_T(k)$ vs k in Fig. 13 for $\lambda=0$ and $\lambda=1$.

At low temperatures, the height of the static structure factor peak is inversely proportional to the density of the kinks whereas the width is directly proportional to the kink density. As soon as we turn on the interaction, the kink density increases. That is why in the presence of interaction ($\lambda=1$), the peak is smaller in height and broader compared to the free ($\lambda=0$) static structure factor peak. Furthermore, we plot in Fig. 14 the total static structure factor $S_T(k)$ vs k for two different temperatures. We find that as we raise the temperature, the peak decreases in height and becomes broad. This is precisely what we expect because the kink density increases with the increase in temperature.

VIII. DISCUSSION

We have developed in this paper a procedure for treating highly nonlinear field configurations like kinks on an equal footing with standard linear configurations like phonons. Some general features of this procedure could, in principle, be extended to the case of higher-dimensional systems. The key point, of course, is the identification of nontrivial local solutions of the field equations in higher dimensions. It seems likely that for systems in metastable equilibrium these ideas may be useful in treating the nucleation problem. It is also

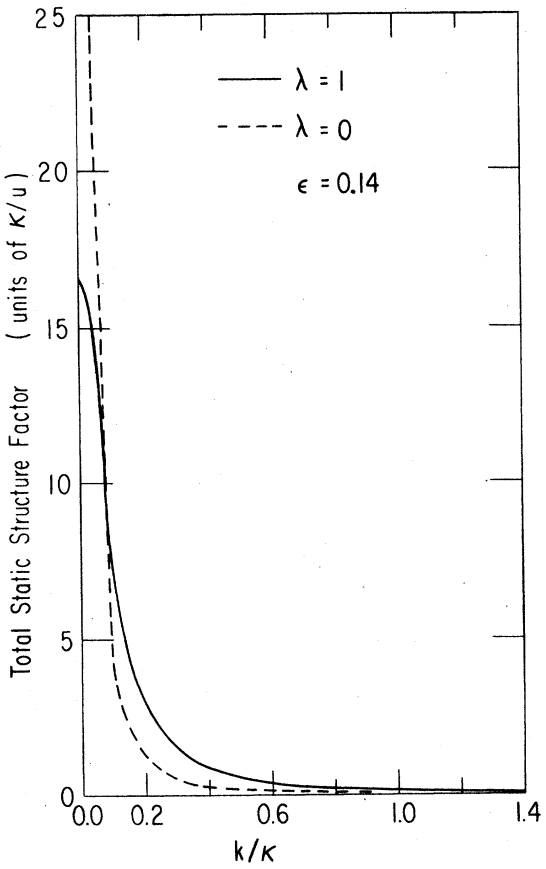

FIG. 13. Total static structure factor $S(k)$ vs k at $\epsilon = 0.14$ for $\lambda = 0$ (dashed line) and $\lambda = 1$ (straight line).

possible that this type of development may be useful in understanding the coexistance region in fluids in three dimensions. We are currently investigating these possibilities.

In a second paper in this series we will indicate how the methods developed in this paper can be used to treat dynamical problems.

ACKNOWLEDGMENT

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APPENDIX

In this Appendix we develop perturbation theory about a single kink. Consider the partition function given in Eq. (2.3),

$$Z = \int \mathfrak{D}\varphi e^{-\beta A\{\varphi\}} . \tag{A1}$$

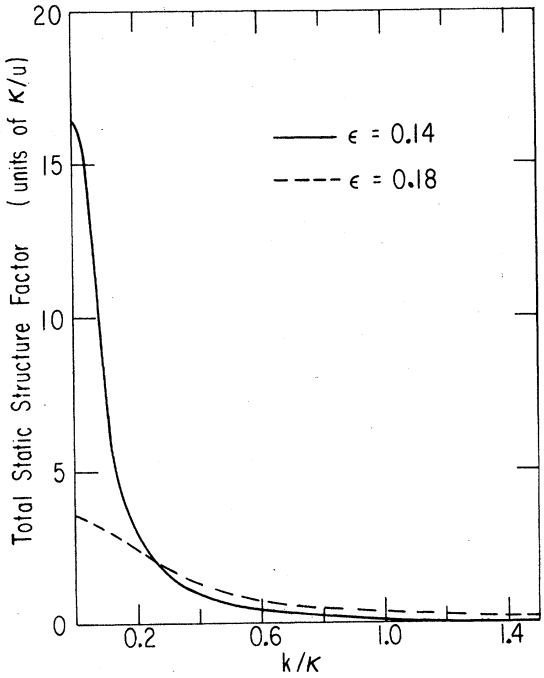

FIG. 14. Total static structure factor $S(k)$ vs k for $\lambda = 1$ at $\epsilon = 0.14$ (straight line) and $\epsilon = 0.18$ (dashed line).

The classical equation for field $\varphi(x)$

$$\frac{\delta A\{\varphi\}}{\delta\varphi(x)} = 0 \tag{A2}$$

possesses the so-called kink solution

$$\varphi_0(x) = (\kappa/\sqrt{u}) \tanh(\kappa/\sqrt{2})(x - X_0) . \tag{A3}$$

We note, however, that the kink depends on the arbitrary "position" X_0. Thus we have a family of solutions of Eq. (A2). For each $\varphi(x)$ we want to choose that solution (or choice of X_0) for which $\varphi(x)$ is best approximated by $\varphi_0(x - X_0)$ near x. We therefore demand that the mean-square deviation

$$D[\varphi; X_0] = \int dx\, [\varphi(x) - \varphi_0(x)]^2 \tag{A4}$$

be a minimum as a function of X_0. Assume that $\bar{X}_0(\varphi)$ is the value of X_0 that minimizes D. We can then introduce the identity

$$\int dX_0\, \delta(X_0 - \bar{X}_0(\varphi)) = 1 , \tag{A5}$$

into our functional integral (A1),

$$Z = \int \mathfrak{D}\varphi \int dX_0\, \delta(X - \bar{X}_0(\varphi)) e^{-\beta A\{\varphi\}} . \tag{A6}$$

We can now expand $A(\varphi)$ around a single kink using

$$\varphi(x)=\varphi_0(x)+\chi(x)\,, \tag{A7}$$

and evaluate the partition function without any problem. This procedure is essentially equivalent to the Faddeev-Popov quantization prescription.

We note that the condition determining $X_0(\varphi)$ is

$$\delta(X_0-X_0(\varphi))=\delta\left(\frac{\partial}{\partial X_0}D[X_0,\varphi]\right)\left|\frac{\partial^2}{\partial X_0^2}D[X_0,\varphi]\right|. \tag{A8}$$

Then

$$\frac{\partial}{\partial X_0}D[X_0,\varphi]=2\int dx\,[\varphi(x)-\varphi_0(x)]\frac{\partial\varphi_0}{\partial x} \tag{A9}$$

and

$$\frac{\partial^2}{\partial X_0^2}D[X_0,\varphi]=2\int dx\left[\left(\frac{\partial\varphi_0}{\partial x}\right)^2-[\varphi(x)-\varphi_0(x)]\frac{\partial^2\varphi_0(x)}{\partial x^2}\right]. \tag{A10}$$

From (A9) we see that the condition that D is a minimum essentially enforces that $\chi(x)$ is orthogonal to $\partial\varphi_0(x)/\partial x$. From a mathematical point of view we could have motivated our constraint condition from the necessity of this orthogonality. We can see this as follows. Suppose that we had proceeded blindly and expanded φ about φ_0 assuming χ to be small. Then we have

$$\begin{aligned}A\{\varphi_0+\chi\}&=A_0\{\varphi_0\}+\frac{1}{2}\frac{\delta^2A\{\varphi\}}{\delta\varphi(x)\delta\varphi(x')}\bigg|_{\varphi=\varphi_0}\chi(x)\chi(x')\\&\quad+O(\chi^3)\\&=A_0\{\varphi_0\}\\&\quad+\frac{1}{2}\int dx\,dx'\,\chi(x)M(x,x')\chi(x')\\&=A_0\{\varphi_0\}+A_0'\{\chi\}\,,\end{aligned} \tag{A11}$$

where the matrix $M(X,X')$ is given by

$$\left(-\frac{\partial^2}{\partial x^2}-\kappa^2+3\kappa^2\tanh^2\frac{\kappa}{\sqrt{2}}(x-X_0)\right)\delta(x-x')=M(x-x')\,. \tag{A12}$$

Then our functional integral (A1) reduces to a Gaussian functional integral

$$Z=e^{-\beta A_0\{\varphi_0\}}\int\mathfrak{D}\chi e^{-A_0'\{\chi\}/2}. \tag{A13}$$

We can evaluate the Gaussian integral by solving for the eigenvalues ϵ_n and eigenfunction $\psi_n(x)$,

$$\int d\bar{x}\,M(x,\bar{x})\psi_n(\bar{x})=\epsilon_n\psi_n(x)\,, \tag{A14}$$

and writing

$$\chi(x)=\sum_n\xi_n\psi_n(x)\,, \tag{A15}$$

so that

$$A_0'\{\chi\}=\sum_n\xi_n^2\epsilon_n. \tag{A16}$$

We have used the orthonormality condition of eigenfunctions to obtain (A16),

$$\int dx\,\psi_n(x)\psi_{n'}(x)=\delta_{nn'}. \tag{A17}$$

Then

$$\begin{aligned}Z&=Je^{-\beta A_0\{\varphi_0\}}\int\prod_{n=0}^{\infty}d\xi_n\exp\left(-\frac{1}{2}\sum_n\xi_n^2\epsilon_n\right)\\&=Je^{-\beta A_0\{\varphi_0\}}\prod_{n=0}^{\infty}\left(\frac{2\pi}{\epsilon_n}\right)^{1/2},\end{aligned} \tag{A18}$$

where the Jacobian J is given as

$$J=\left|\frac{\mathfrak{D}[\chi]}{\mathfrak{D}[\xi]}\right|. \tag{A19}$$

The problem with this procedure is that there is an eigenfunction with zero eigenvalue;

$$\psi_0(x)=\frac{\partial\varphi_0(x)}{\partial x}\Big/\left|\frac{\partial\varphi_0}{\partial x}\right|=\frac{\kappa^2}{(2uC)^{1/2}}\frac{1}{\cosh^2(\kappa x/\sqrt{2})}\,, \tag{A20}$$

where

$$\left|\frac{\partial\varphi_0}{\partial\kappa}\right|^2=C=2\sqrt{2}\kappa^3/3U. \tag{A21}$$

This zero eigenfunction arises due to the translational invariance in the system and is a general feature of classical solutions. We see this by noticing that if $\varphi_0(\chi)$ is a classical solution,

$$\frac{\delta A\{\varphi_0\}}{\delta\varphi_0(\chi)}=0\,, \tag{A22}$$

so also is $\varphi_0(x-X_0)$,

$$\frac{\delta A\{\varphi_0\}}{\delta\varphi_0(x-X_0)}=0. \tag{A23}$$

Differentiate (A23) with respect to X_0 to find that

$$\frac{\partial}{\partial X_0}\frac{\delta A\{\varphi_0\}}{\delta\varphi_0(x-X_0)}=\int dx'\frac{\delta A\{\varphi_0\}}{\delta\varphi_0(x-X_0)\delta\varphi_0(x'-X_0)}\times\frac{\partial\varphi_0(x'-X_0)}{\partial X_0}=0 \tag{A24}$$

or

$$\int dx'\,M(x,x')\frac{\partial\varphi_0}{\partial x'}=0\,, \tag{A25}$$

implies that $\partial\varphi_0(x)/\partial x$ corresponds to an eigen-

function of M with zero eigenvalue. The integral is not defined without the constraint. With our choice of constraint we demand χ to be orthogonal to zero eigenfunction and the integral over ξ_0 can be treated as a δ-function integral. Then the partition function Z can be written as

$$Z = e^{-\beta A_0\{\varphi_0\}}\sqrt{C}\int \mathfrak{D}\chi \int dX_0 \times \delta\Big(\int dx\,\chi(z)\psi_0(x)\Big) e^{-\beta A_0'\{\chi\}} = e^{-\beta A_0\{\varphi_0\}} Z', \tag{A26}$$

where

$$Z' = J\sqrt{C}\int \prod_{n=0}^{\infty} d\xi_n\,\delta(\xi_0)\int dX_0 \exp\Big(-\sum_{n=0}^{\infty}\xi_n^2\epsilon_n\beta\Big) = J\sqrt{C}\,V\prod_{n=1}^{\infty}\left(\frac{2\pi}{\epsilon_n\beta}\right)^{1/2}. \tag{A27}$$

The energy eigenvalues ϵ_n can be obtained by solving Eq. (A14),

$$\epsilon_0 = 0\,,\quad \epsilon_1 = \tfrac{3}{2}\kappa^2\,,\quad \epsilon_k = (k^2+4)\tfrac{1}{2}\kappa^2\,, \tag{A28}$$

and the density of the continuum states is given by[24]

$$\frac{dn}{dk} = \frac{1}{2\pi}\left[\frac{\kappa(2L)}{\sqrt{2}} - \frac{6(k^2+2)}{(k^2+1)(k^2+4)}\right]. \tag{A29}$$

Then we consider

$$\frac{Z'}{Z_0} = \sqrt{A}\,V\left(\frac{2\pi}{\epsilon_1}\right)^{1/2} Q\,, \tag{A30}$$

where Z_0 is the partition function in the absence of kink. The factor Q is given as

$$Q = \prod_{S=2}^{\infty}\frac{1}{(\epsilon_S/\pi)^{1/2}}\prod_{k=0}^{\infty}\left(\frac{\epsilon_k^0}{\pi}\right)^{1/2} = \exp\left[\sum_S \ln\left(\frac{\pi}{\epsilon_S}\right)^{1/2} + \sum_k \ln\left(\frac{\epsilon_k^0}{\pi}\right)^{1/2}\right] = \exp\left[\frac{1}{2}\int_0^{\infty} d\epsilon\,[\rho^0(\epsilon)-\rho(\epsilon)]\ln\left(\frac{\epsilon}{\pi}\right)\right], \tag{A31}$$

where

$$\epsilon = \tfrac{1}{2}\kappa^2(4+k^2)$$

and

$$\rho^0(k) - \rho(k) = \frac{6(k^2+2)}{2\pi(k^2+1)(k^2+4)}\,. \tag{A32}$$

Then

$$Q = \exp\left[\tfrac{1}{2}\ln\left(\frac{\kappa^2}{2\pi}\right)\int_{-\infty}^{\infty} dk\,[\rho^0(k)-\rho(k)] + \frac{1}{2}\int_{-\infty}^{\infty} dk\,[\rho^0(k)-\rho(k)]\ln(4+k^2)\right] = \frac{\kappa^2}{2\pi}\exp\left(\frac{3}{2\pi}\int_{-\infty}^{\infty} dk\,\frac{k^2+2}{(k^2+1)(k^2+4)}\ln(4+k^2)\right). \tag{A33}$$

With a little algebra, one can show that the integral appearing in (33) is equal to $\frac{2}{3}\pi\ln 12$. Then

$$Q = \frac{\kappa^2}{2\pi}\exp\left(\frac{3}{2\pi}I\right) = \frac{\kappa^2}{2\pi}\exp\left(\frac{3}{2\pi}\frac{2\pi}{3}\ln 12\right) = \frac{6\kappa^2}{\pi}\,. \tag{A34}$$

Then

$$\frac{Z'}{Z_0} = \sqrt{C}\,V\left(\frac{2\pi}{\epsilon_1\beta}\right)^{1/2}\frac{6\kappa^2}{\pi}\beta. \tag{A35}$$

Substitute $\epsilon_1 = \frac{3}{2}\kappa^2$ and (A21) in (A35) to obtain

$$Z'/Z_0 = V\kappa(32\sqrt{2}/\pi\epsilon)^{1/2}. \tag{A36}$$

Then the contribution to the partition function from a single kink is

$$Z_K = e^{-\beta A_0\{\varphi_0\}}Z' = Z_0 V\kappa\left(\frac{32\sqrt{2}}{\pi\epsilon}\right)^{1/2}\exp[-\beta(E_K + E_{\rm vac})]\,. \tag{A37}$$

This is the single-kink contribution to the partition evaluated to lowest order in the coupling [in Eq. (A11) we kept only the Gaussian terms]. We could follow Gervais and Sakita[16] and develop a perturbation theory expansion giving the corrections to (A37) as a power series in ϵ. One can show, following work due to Lazarides[28] in treating metastable systems, that this series is, again, non-Borel summable because of the existence of a real pseudoparticle. This real pseudoparticle corresponds to an indirect manifestation of the original kink.

[1] T. Schneider and E. Stoll [Phys. Rev. B 13, 1216 (1976)] discuss various models and the corresponding significance of associated parameters.

[2] J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B 11, 3535 (1975).

[3] T. Schneider and E. Stoll, Phys. Rev. Lett. 35, 296 (1975).

[4] J. R. Koehler, A. R. Bishop, J. A. Krumhansl, and J. R. Schrieffer, Solid State Commun. 17, 1515 (1975).

[5] J. S. Langer, Ann. Phys. (N.Y.) 41, 108 (1967); Phys. Rev. Lett. 14, 973 (1968); Ann. Phys. (N.Y.) 54, 258 (1969); Ann. Phys. (N.Y.) 65, 53 (1971); J. S. Langer

and M. Barron, Ann. Phys. (N. Y.) 78, 421 (1973); J. S. Langer, Acta Metall; 21, 1649 (1973); J. S. Langer and L. A. Turski, Phys. Rev. A 8, 3230 (1973); J. S. Langer, Physica 73, 61 (1974).
[6]S. Coleman, Phys. Rev. D 15, 2929 (1977).
[7]C. G. Callen, Jr. and S. Coleman, Phys. Rev. D 16, 1762 (1977).
[8]P. H. Frampton, Phys. Rev. Lett. 37, 1378 (1976); Phys. Rev. D 15, 2922 (1977).
[9]L. N. Lipatov, JETP Lett. 24, 157 (1976).
[10]E. Brézin, J. C. LeGuillou, and J. Zinn-Justin, Phys. Rev. D 15, 1544 (1977). (For a review, see E. Brézin, The Role of Instantons in Divergent Perturbation Series, European Particle Physics Conference, July, 1977.)
[11]E. Brézin, J. C. LeGuillou, and J. Zinn-Justin, Phys. Rev. D 15, 1558 (1977).
[12]E. Brézin, G. Parisi, and J. Zinn-Justin, Phys. Rev. D 16, 408 (1977).
[13]V. L. Berezinskii, Zh. Eksp. Teor. Fiz. 59, 907 (1970) [Sov. Phys. JETP 32, 493 (1971)]; J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973).
[14]In the two-dimensional planar model vortices tend to suppress the transition temperature relative to that for higher-dimensional systems. However, the formation of single vortices is energetically unfavorably at zero temperature. The result is that the system does not undergo the usual type of phase transition. Instead there is a temperature T_c below which vortices appear only in pairs. Thus as one approaches T_c from below one finds a transition due to dissociation of pairs. There is, however, in this case, no spontaneous symmetry breaking.
[15]There are examples of both classes in non-Abelian gauge theories. Instantons have finite action and short-range interactions while so-called merons are similar to the vortices in the planar mode. [See, C. B. Callan, Jr., R. Dashen, and D. J. Gross, Phys. Lett. B 66, 375 (1977).]
[16]J. L. Gervais and B. Sakita, Phys. Rev. D 11, 2943 (1975).
[17]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Addison-Wesley, Reading, Mass., 1958), pp. 176–178.
[18]This restriction in the low-temperature phase is treated in a convincing manner by J. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B 16, 1217 (1977).
[19]A. M. Polyakov, Nucl. Phys. B 120, 429 (1977).
[20]D. J. Scalapino, M. Sears, and R. A. Ferrell, Phys. Rev. B 6, 3409 (1972).
[21]T. Riste, E. J. Samuelson, K. Otens, and J. Feder, Solid State Commun. 9, 1455 (1971); W. Cochran, Adv. Phys. 9, 387 (1960); G. Shirane and J. D. Axe, Phys. Rev. Lett. 27, 1803 (1971); S. M. Shapiro, J. D. Axe, G. Shirane, and T. Risle, Phys. Rev. B 6, 4332 (1972); J. F. Scott, Rev. Mod. Phys. 46, 83 (1974).
[22]E. Brézin, D. S. Wallace, and K. G. Wilson, Phys. Rev. B 7, 232 (1973).
[23]D. J. Amit and M. Zannetti, J. Stat. Phys. 7, 31 (1973).
[24]For a thorough discussion, see, R. F. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. D 10, 4114 (1974); 10, 4130 (1974); 10, 4138 (1974); R. Rajaraman, Phys. Rep. C 21, 227 (1975).
[25]We will use the word "instanton" to describe pseudoparticles localized in space. This nomenclature first arose in field theory where field configurations were found to be localized in 3 space and one-time dimensions. Thus these events occur only for an "instant" in time.
[26]Here we simply paraphrase the discussion of Brézin, in Ref. 10.
[27]S. Graffi and V. Grecchi, Phys. Rev. D 8, 3487 (1973).
[28]G. Lazarides (unpublished).
[29]T. Ohta and K. Kawasaki, Prog. Theor. Phys. 58, 467 (1977).
[30]E. Gildner and A. Pastrascioiu, Phys. Rev. D 16, 423 (1977).
[31]H. Neuberger (unpublished).
[32]I. M. Gel'fand and A. M. Yaglom, J. Math. Phys. 1, 48 (1960).
[33]R. Rajaraman, Phys. Rev. D 15, 2866 (1977).
[34]S. Aubry, J. Chem. Phys. 62, 3217 (1975).