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Statistical mechanics of one-dimensional solitary-wave-bearing scalar fields: Exact results and ideal-gas phenomenology

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The statistical mechanics of one-dimensional scalar fields governed by nonlinear wave equations having solitary-wave (soliton) solutions are discussed in detail. Previously neglected "phase-shift" interactions between phonons and solitary waves (kinks) are taken into account and it is shown that these interactions provide the mechanism for sharing of energy and degrees of freedom among the "elementary" excitations of the nonlinear system. In particular, the ideal-gas phenomenology proposed by Krumhansl and Schrieffer for the "ϕ^4" model is corrected and extended to the entire class of nonlinear Klein-Gordon models having solitary-wave solutions (e.g., ϕ^4, sine-Gordon, double-quadratic, etc.). By a comparison of the results of the phenomenological approach to those obtained via the exact transfer-operator method, it is found that the ideal-gas phenomenology gives *exact* results for the various low-temperature thermodynamic functions and correlation lengths.

I. INTRODUCTION

Recently there has been a remarkable surge of interest in condensed-matter systems described by one-dimensional nonlinear scalar fields governed by nonlinear energy functionals.[1] The governing equations frequently admit large-amplitude localized field profiles which are physically distinct from those obtainable by superposition of small-amplitude or "linearized" profiles. Frequently these localized large-amplitude excitations can propagate through the system without distortion of shape and are commonly referred to as *solitary waves*. They exhibit remarkable stability and other particlelike properties. (If they retain their identity after collisions, they are called *solitons*.[2]) Indeed, because of their localized nature, they have found widespread use as one-dimensional models of extended particles in nonlinear quantum-field theories,[3] dislocations in crystals,[4] planar domain walls in ferromagnets[5] and ferroelectrics,[6] propagating flux quanta in Josephson transmission lines,[7] disgyration planes[8] in superfluid ^{3}He, charge carriers in weakly pinned charge-density-wave condensates,[9] and charged dislocations[10] in superionic conductors, to mention only a few examples.

In anharmonic systems where the number of nonlinear excitations present is thermally controlled,[6,9,10] it is important to investigate the statistical mechanics of the field in order to determine their thermal density as well as their contribution to correlation functions and other thermodynamic quantities. In a general investigation one would first identify natural elementary excitations, including the nonlinear solitary waves. If these are known, it is then physically and mathematically advantageous to carry out the calculation of the partition function in a representation treating these excitations as distinct nonlinear modes.

In this paper we discuss a class of solitary-wave-bearing Hamiltonians for which this approach can be pursued analytically. We have included the effect of *interactions* between the elementary excitations and find that this leads to "free-energy sharing" among the excitations. These interactions are essential for a correct interpretation of results available from a transfer-operator evaluation of the partition function. This approach provides considerable insight which should be of use in analyzing the role of nonlinear excitations in the statistical mechanics of more complex systems.

This investigation was initiated by Krumhansl and Schrieffer[6] (KS) who studied the statistical mechanics of a scalar field in a so-called "ϕ^4" or "double-well" potential[3,6] as a simple model of a one-dimensional ferroelectric. Using the transfer integral method discussed by Scalapino, Sears, and Ferrell,[11] KS were able to calculate the classical partition function (and hence the free energy) exactly. Moreover, they calculated the same free energy phenomenologically at low temperatures assuming an "ideal gas" of completely non-

interacting solitary waves (kinks) and small amplitude "phonon" excitations and found reasonable agreement with the exact results of the transfer integral approach. They were thus able to identify terms in the free energy as arising from either the kinks or the phonons. This led KS to propose that the nonlinear solitary waves can be regarded as "elementary" excitations. The inclusion of interactions (in the form of residual phase-shift interactions neglected by KS) between the kinks and phonons allows us to obtain precise agreement between the phenomenology and the exact results.

Recently, the concepts and methods of KS have been extended to cases where the "potential" for the field is periodic (and hence bounded) as opposed to the unbounded ϕ^4 potential treated by KS. The transfer integral technique can be applied to periodic potentials; Gupta and Sutherland[12] have studied the potential $V(\phi)=1-\cos\phi$ in particular, finding sine-Gordon (SG) solitons[2] as the elementary "kink" excitations. Currie, Fogel, and Palmer[13] have analyzed the exact results[12] from an ideal-gas viewpoint and find that this viewpoint is natural and consistent with exact results; moreover, solitons and "phonons" were found to "share" free energy (and internal energy) in much the same manner as that which occurs for the ϕ^4 case. We shall show below that in the general case this sharing results from phase-shift interactions between the kinks (solitons) and phonons. Indeed, the ϕ^4 kinks and SG solitons share the remarkable property that they simply shift the phases of extended linear excitations without reflection; as a consequence, the role of kink-phonon interactions in the statistical mechanics can be identified quite easily.

Although the ϕ^4 and SG systems provide especially tractable cases for studying the role of kink-phonon interactions in the statistical mechanics of solitary-wave-bearing systems, it is by no means necessary to restrict oneself to such "reflectionless" cases. In addition to treating these particular cases we also describe a simple system possessing kink solutions which are not perfectly transparent to phonons, namely, the double-quadratic (DQ) system which is obtained by replacing the ϕ^4 double well with a double well consisting of two displaced parabolas. Thus, the ϕ^4, DQ and SG cases span a large variety of potentials [unbounded (ϕ^4, DQ), bounded (SG), transparent (ϕ^4, SG), nontransparent (DQ)], and as such these three cases serve as prototypical models for a large class of solitary-wave-bearing potentials.

The sine-Gordon case is an integrable system for which a Hamiltonian can be constructed with pieces corresponding to solitons, breathers, and phonons as bona fide elementary excitations. A canonical transformation[14] achieves such a separation, and the contribution of each type of excitation to the free energy can, in principle, be calculated (with due regard for phase-shift interactions and their modification of the phonon density of states). The ϕ^4 and DQ Hamiltonians are *not* rigorously separable as is that of SG, but the phenomenological results obtained by *assuming* separability at low temperature can be verified by comparison with corresponding exact transfer integral results, suggesting that separability is approximately valid at low temperature for the *entire* class of Hamiltonians considered.

In Sec. II we define a general class of solitary-wave-bearing one-dimensional Hamiltonians. We use transfer integral techniques to examine the exact statistical mechanics for this class, and we present the low-temperature asymptotic results for the ϕ^4, DQ, and SG cases. In Sec. III, we consider the phenomenological approach to calculating free energies, etc., based on the role of kink-phonon interactions in the free-energy-sharing process. Exact agreement with transfer-operator results is obtained at low temperatures. Section IV deals with the sine-Gordon case in terms of its separability properties, and a discussion is given of the problems we have encountered in an attempt to include SG "breather" excitations in the phenomenology. In Sec. V we examine equilibrium correlation functions and the role of solitary waves in determining low-temperature correlation lengths. Finally, in Sec. VI we present our conclusions and discuss extensions of the theory.

II. EXACT STATISTICAL MECHANICS FOR A CLASS OF NONLINEAR HAMILTONIANS

In this section we consider the classical statistical mechanics of a general class of nonlinear Hamiltonians having kink or soliton excitations. The class is restricted here to one-component fields defined (initially) on one-dimensional lattices (some generalizations are possible[15-18]) and has the following form:

$$\mathcal{H}=\sum_i lA\left(\tfrac{1}{2}\dot{\phi}_i^2+\frac{1}{2}\frac{c_0^2}{l^2}(\phi_{i+1}-\phi_i)^2+\omega_0^2 V(\phi_i)\right), \quad (2.1)$$

where $\{\phi\}$ is a one-component dimensionless field defined on a one-dimensional lattice of points (labeled by i) with lattice constant l. The first term represents the kinetic energy carried by the field, the second represents harmonic coupling ("strain" energy) between field values at

neighboring lattice sites and the last term an "on-site" or external potential depending only on the field and not explicitly on lattice position. The constant c_0 is a characteristic velocity and ω_0 a characteristic frequency. The constant A sets the energy scale and has dimensions of (energy) × (length)$^{-1}$ × (time)^2.

It is important to distinguish two quite different regimes according to whether the length $d \equiv c_0/\omega_0$ is on the order of the lattice constant l or large compared to l. The first results when the interaction energy between neighbors is small compared to the on-site potential and is termed the "order-disorder" limit, since field values on neighboring sites can fluctuate (thermally) almost independent of one another. In the opposite limit ($d \gg l$), the coupling between sites is strong enough to ensure that variations of ϕ from site to site are quite small, at least at low temperatures. In this "displacive" limit we may replace the site index i by a continuous position variable x so that ϕ becomes a continuous function of x and t, $\phi = \phi(x,t)$. Although the order-disorder limit is a physically interesting case (e.g., Ising), we shall restrict ourselves to the displacive limit where nonlinear kinks become well-defined[19] elementary excitations with long lifetimes and as such behave[20] very much like particles.

In the continuum (displacive) limit the Hamiltonian (2.1) is transformed approximately to

$$\mathcal{H} = A \int dx \{ \tfrac{1}{2}[\dot{\phi}(x,t)]^2 + \tfrac{1}{2}c_0^2[\phi_x(x,t)]^2 + \omega_0^2 V(\phi) \}, \tag{2.2}$$

where $\phi_x(x,t) = (\partial/\partial x)\phi(x,t)$ replaces the finite difference $(\phi_{i+1} - \phi_i)/l$. We shall have occasion to employ both forms [(2.1) and (2.2)] of the Hamiltonian for the system. The discrete form (2.1) is used in obtaining exact statistical mechanical results via the transfer-operator formalism, whereupon the explicit process of taking the continuum limit follows. The continuum form (2.2) is used to study the nature of the solitary-wave (kink) and linear (phonon) excitations of the system; these excitations arise as solutions to the Euler-Lagrange equation of motion following from Eq. (2.2):

$$\ddot{\phi} - c_0^2\phi_{xx} + \omega_0^2 \frac{dV}{d\phi} = 0. \tag{2.3}$$

The *only* restriction on the local dimensionless potential $V(\phi)$ is that it have at least two *degenerate* minima ($V = 0$) at, for example, $\phi = \phi_1$ and $\phi = \phi_2$ (see Fig. 1). This is sufficient to admit elementary solitary-wave (kink) solutions $\phi_K^{(v)}$ to Eq. (2.3). We look for a kink moving with velocity v and impose appropriate boundary conditions,

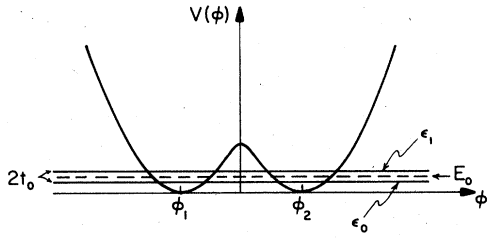

FIG. 1. Schematic plot of a double-well on-site potential. The lowest two eigenvalues of Eq. (2.23) are represented by the horizontal solid lines. These two eigenvalues are symmetrically tunnel-split (total splitting $= 2t_0$) from the lowest level E_0 of an isolated harmonic well. The height of E_0 above the potential minimum and the magnitude of the splitting are greatly exaggerated for clarity.

viz, $d\phi_K^{(v)}(s)/ds(s = \pm\infty) = 0$, $V(\phi_K^{(v)}(s = \pm\infty)) = 0$ (a convenient energy zero), $\phi_K^{(v)}(s = \pm\infty) = \phi_{1,2}$ with $s \equiv x - vt$. The solution is obtained from the first integral of Eq. (2.3),

$$\frac{d\phi_K^{(v)}}{ds} = \pm\left[\frac{2\omega_0^2}{c_0^2}\left(1 - \frac{v^2}{c_0^2}\right)^{-1} V(\phi_K^{(v)})\right]^{1/2}, \tag{2.4}$$

by integrating a second time:

$$x - vt = \pm\left(1 - \frac{v^2}{c_0^2}\right)^{1/2} \frac{d}{\sqrt{2}} \int_{\phi_K^{(v)}(0)}^{\phi_K^{(v)}(x-vt)} d\phi\,[V(\phi)]^{-1/2}. \tag{2.5}$$

Equation (2.5) provides an implicit solution for $\phi_K^{(v)}$ as a function of $x - vt$. The "relativistic" dependence on v follows from the covariant form of Eq. (2.3) and appears again in the energy, E_K, associated with a single kink:

$$E_K^{(v)} = E_K^{(0)}(1 - v^2/c_0^2)^{-1/2} \tag{2.6a}$$

$$= (E_K^{(0)2} + p^2c_0^2)^{1/2}, \tag{2.6b}$$

where $p = M_K v(1 - v^2/c_0^2)^{-1/2}$ is the relativistic momentum and $E_K^{(0)}$ is the rest energy of the kink:

$$E_K^{(0)} = M_K c_0^2. \tag{2.7}$$

The kink rest mass M_K is given by

$$M_K = \frac{2A}{d^2} \int_{-\infty}^{+\infty} dx\, V[\phi_K^{(0)}(x)] \tag{2.8}$$

$$= \frac{\sqrt{2}A}{d} \int_{\phi_1}^{\phi_2} d\phi\, |V(\phi)|^{1/2}. \tag{2.9}$$

In Fig. 2, we plot a schematic kink solution (2.5) in its rest frame. The kink carries the field from

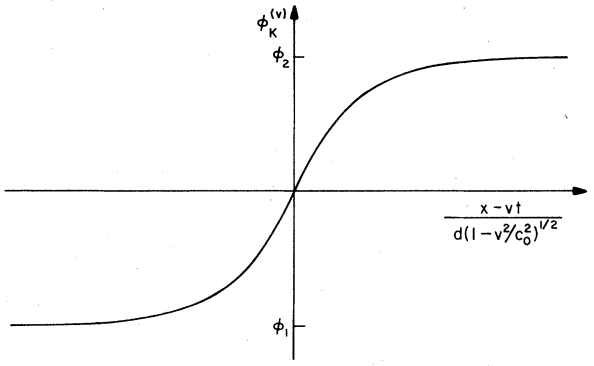

FIG. 2. Schematic waveform of a traveling kink $\phi_K^{(v)}$ viewed in its rest frame. An antikink waveform can be obtained by reflection through the horizontal axis.

one minimum (ϕ_1) of the local potential (see Fig. 1) to another (ϕ_2) or vice versa (antikink), over a "kink width" given roughly by $2d$. It is worth noting that if $V(\phi)$ has sufficient structure, more than one type of kink may be possible.[21] At low temperatures one may obtain a dikink[22] or polykink ideal gas using the same formalism developed below for a monokink (plus antikink) gas.

Familiar analytic results for ϕ^4 and SG potentials are readily retrieved from Eqs. (2.5) and (2.9), and Table I shows the local potential, kink solution, and kink rest energy for these two special cases, as well as for the double-quadratic (DQ) potential (see below). The stability of these one-dimensional kinks against internal perturbations is guaranteed on grounds of topological stability[23] or by explicit calculation (see below).

The other significant excitations are quite different in character and physical significance from the large-amplitude, spatially localized kinks, namely, the approximate, small-amplitude, extended harmonic solutions (phonons) to Eq. (2.3) when linearized with respect to a potential minimum:

$$\phi(x,t)-\phi_{1,2}\propto\exp[i(kx-\omega_k t)]\,, \tag{2.10}$$

with the continuum dispersion relation

$$\omega_k^2=\omega_0^2+c_0^2k^2\,. \tag{2.11}$$

In writings Eqs. (2.10) and (2.11), we have assumed for simplicity that $V(\phi)$ is symmetric $[V(-\phi)=V(\phi)]$ and has been scaled so that

$$\left.\frac{d^2V}{d\phi^2}\right|_{\phi_{1,2}}=1 \tag{2.12}$$

in the harmonic approximation.

In Sec. III it will be necessary to replace the continuum (Debye) dispersion (2.11) with that appropriate for the discrete lattice:

$$\omega_k^2=\omega_0^2+4(c_0/l)^2\sin^2(\tfrac{1}{2}lk)\,. \tag{2.13}$$

The lattice parameter l appears in the free-energy expression obtained phenomenologically as well as in the exact free energy for the discrete lattice, as we show presently. One can then compare these two results in the limit as the ratio l/d is explicitly taken to zero.

We now consider the exact calculation of the one-dimensional classical partition function for discrete systems governed by the Hamiltonian given in Eq. (2.1) above. We shall be particularly interested in the low-temperature free-energy, correlation functions, etc., in the continuum limit (as $l/d\to 0$) where we expect to identify kink and phonon contributions separately. The use of a transfer integral operator technique for this purpose has already been well documented.[6,11-13] The classical partition function factors

$$Z=Z_\phi Z_\Phi\,, \tag{2.14}$$

with

$$Z_\phi=(2\pi Al/\beta h^2)^{N/2} \tag{2.15}$$

and

$$Z_\Phi=\sum_n\exp(-\beta A\omega_0^2L\epsilon_n)\,, \tag{2.16}$$

where $\beta\equiv(k_BT)^{-1}$, h is Planck's constant, and $L=Nl$ is the total length of the system of N particles with assumed periodic boundary conditions: $\phi_{N+1}=\phi_1$. Of course, other types of boundary conditions may be appropriate as dictated by the particular physical context. The quantities ϵ_n appearing in Eq. (2.16) for the "configurational" partition function Z_Φ are the eigenvalues of the transfer integral operator defined by

$$\int_{-\infty}^{+\infty}d\phi_i\exp[-\beta lA\omega_0^2f(\phi_{i+1},\phi_i)]\Phi_n(\phi_i)$$
$$=\exp(-\beta lA\omega_0^2\epsilon_n)\Phi_n(\phi_{i+1})\,, \tag{2.17}$$

where

$$f(\phi_{i+1},\phi_i)\equiv\frac{1}{2}\frac{d^2}{l^2}(\phi_{i+1}-\phi_i)^2$$
$$+\tfrac{1}{2}[V(\phi_i)+V(\phi_{i+1})]\,. \tag{2.18}$$

The eigenfunctions $\{\Phi_n\}$ constitute a complete orthonormal set on the interval $\phi\subset(-\infty,+\infty)$.

In the thermodynamic limit ($N\to\infty, L\to\infty$, $L/N=l$ constant), Z_Φ is dominated by the lowest eigenvalue ϵ_0, so that the configurational (i.e., potential energy) contribution to the free-energy density $F\,[\equiv-(k_BT/L)\ln Z]$ becomes

$$F_\Phi\xrightarrow[L\to\infty]{}A\omega_0^2\epsilon_0\,. \tag{2.19}$$

TABLE I. Various quantities for the ϕ^4, sine-Gordon (SG), and double-quadratic (DQ) systems. $V(\phi)$ is the local on-site potential, $\phi_K^{(v)}(x,t)$ is the traveling kink (+) or antikink (–) solution, $E_K^{(0)}$ is the rest energy of the kink (or antikink), $V''(\phi_K^{(0)}(x))$ is the potential appearing in the Schrödinger-like equation for small oscillations about the kink, $f_{b,n}(x)$ are the bound states of $V''(\phi_K^{(0)}(x))$, $f_k(x)$ are the scattering states, and $\Delta(k)$ is the phase shift of $f_k(x)$ (see Ref. 33 for special handling of the DQ case). The quantity σ appears in the kink self-energy [Eq. (3.32)] and B is the phase-space reduction factor [Eq. (3.24a)].

	ϕ^4	SG	DQ
$V(\phi)$	$\frac{1}{8}(\phi^2-1)^2$	$1-\cos\phi$	$\frac{1}{2}(\lvert\phi\rvert-1)^2$
$\phi_K^{(v)}(x,t)$	$\tanh\left(\pm\dfrac{x-vt}{2d(1-v^2/c_0^2)^{1/2}}\right)$	$4\tan^{-1}\left[\exp\left(\pm\dfrac{x-vt}{d(1-v^2/c_0^2)^{1/2}}\right)\right]$	$\pm\mathrm{sgn}(x-vt)\left[1-\exp\left(-\dfrac{\lvert x-vt\rvert}{d(1-v^2/c_0^2)^{1/2}}\right)\right]$
$E_K^{(0)}$	$\frac{2}{3}A\omega_0 c_0$	$8A\omega_0 c_0$	$A\omega_0 c_0$
$V''[\phi_K^{(0)}(x)]$	$1-\frac{3}{2}\mathrm{sech}^2\left(\dfrac{x}{2d}\right)$	$1-2\,\mathrm{sech}^2\left(\dfrac{x}{d}\right)$	$1-\delta(x/2d)$
$f_{b,n}(x)$	$f_{b,1}(x)=\frac{1}{2}\left(\dfrac{3}{2d}\right)^{1/2}\mathrm{sech}^2\left(\dfrac{x}{2d}\right)$ $f_{b,2}(x)=\frac{1}{2}\left(\dfrac{3}{d}\right)^{1/2}\mathrm{sech}\left(\dfrac{x}{2d}\right)\tanh\left(\dfrac{x}{2d}\right)$	$f_{b,1}(x)=\dfrac{1}{\sqrt{2d}}\mathrm{sech}\left(\dfrac{x}{d}\right)$	$f_{b,1}(x)=\dfrac{1}{\sqrt{d}}\exp(-\lvert x\rvert/d)$
$f_k(x)$	$[2\pi(1+d^2k^2)(4+d^2k^2)]^{-1/2}e^{ikx}$ $\times\left(3\tanh^2\dfrac{x}{2d}-6ikd\tanh\dfrac{x}{2d}-(1+4d^2k^2)\right)$	$2\pi(1+d^2k^2)^{-1/2}e^{ikx}\left(kd+i\tanh\dfrac{x}{d}\right)$	$\dfrac{1}{\sqrt{2\pi}}\sin(kx);\quad k<0$ $\dfrac{1}{\sqrt{2\pi}}\dfrac{\cos[kx+\frac{1}{2}\Delta(k)]}{(1+d^2k^2)^{1/2}},\quad k>0,\quad x>0$ $\dfrac{1}{\sqrt{2\pi}}\dfrac{\cos[kx-\frac{1}{2}\Delta(k)]}{(1+d^2k^2)^{1/2}},\quad k>0,\quad x<0$
$\Delta(k)$	$2\pi\dfrac{k}{\lvert k\rvert}-2\tan^{-1}kd-2\tan^{-1}2kd$	$\pi\dfrac{k}{\lvert k\rvert}-2\tan^{-1}kd$	$\pi-2\tan^{-1}kd,\quad k\geq 0$ $0,\quad k<0$
σ	$\ln(2\sqrt{3})$	$\ln(2)$	$\ln(\sqrt{2})$
B	2	1	2

Other equilibrium properties can be calculated[6,11] with the same technique. For instance, the static correlation functions for the field and the squared field are given by

$$C_1(x) \equiv \langle \delta\phi(x)\delta\phi(0)\rangle = \sum_n |\langle n|\delta\phi|0\rangle|^2 \exp[-\beta A\omega_0^2(\epsilon_n-\epsilon_0)x] \tag{2.20}$$

and

$$C_2(x) \equiv \langle \delta\phi^2(x)\delta\phi^2(0)\rangle = \sum_n |\langle n|\delta\phi^2|0\rangle|^2 \exp[-\beta A\omega_0^2(\epsilon_n-\epsilon_0)x], \tag{2.21}$$

respectively, where $\delta\phi(x)\equiv\phi(x)-\langle\phi\rangle$ and $\delta\phi^2(x)\equiv\phi^2(x)-\langle\phi^2\rangle$. At large distances, $C_1(x)$ and $C_2(x)$ are dominated by the state with the smallest eigenvalue for which the corresponding matrix elements are nonvanishing (excluding the $n=0$ terms). It should be noted that if $V(\phi)$ is periodic, a more interesting correlation function is

$$C_{\text{periodic}}(x) \equiv \langle e^{i\phi(x)}e^{-i\phi(0)}\rangle = \sum_n |\langle n|e^{i\phi}|0\rangle|^2 \exp[-\beta A\omega_0^2(\epsilon_n-\epsilon_0)x], \tag{2.22}$$

since the density of kinks at low temperatures can be more easily extracted from this function rather than $C_1(x)$. We return to this point in Sec. V.

The transfer-operator eigenstructure can be obtained under general conditions (displacive or order-disorder) by solving Eq. (2.17) numerically,[11,15] via a renormalization group procedure,[24] etc. However, much more intuition can be fostered from a differential approximation valid when $l/d \ll 1$, i.e., in the displacive limit of slowly varying fields. The Fredholm integral equation (2.17) for $\Phi(\phi)$ can be replaced in this limit by the following eigenvalue equation [(valid to $O(l/d)$] for a related eigenfunction $\psi(\phi)=\exp[-\frac{1}{2}\beta lA\omega_0^2 V(\phi)]\times\Phi(\phi)$:

$$\hat{H}(\phi)\psi_n(\phi)=\epsilon_n\psi_n(\phi), \tag{2.23}$$

where

$$\hat{H}(\phi) = -\frac{1}{2m^*}\frac{d^2}{d\phi^2} + V(\phi) + V_0, \tag{2.24}$$

$$m^* = A^2\omega_0^2 c_0^2\beta^2 \propto (\beta E_K^{(0)})^2, \tag{2.25}$$

and

$$V_0 = (2\beta\omega_0^2 lA)^{-1}\ln(Ac_0^2\beta/2\pi l). \tag{2.26}$$

We are thus faced with a pseudo-Schrödinger equation for a single particle of dimensionless "mass" m^* in one dimension, moving in the nonlinear potential $V(\phi)$. We note that V_0 acts as a temperature-dependent "energy" minimum which is important for free energy, entropy, etc., but not for correlation functions. No real quantum mechanics is involved in Eq. (2.23) ($\hbar$ is replaced essentially by temperature) but intuition from the familiar quantum problem is very helpful.

Physical interpretations of thermodynamic functions following from Z are possible at both high[13] and low temperatures. We shall concentrate here on the low-temperature region, specifically $\beta E_k^{(0)} \gg 1$, where kink excitations play a prominent role. In this regime $m^* \gg 1$, and the eigenspectrum will be "tunnel-split" to remove degeneracy from the eigenstates of individual wells in $V(\phi)$. Referring to Fig. 1, if E_0 is the lowest level in a single isolated well (measured from the minimum V_0), then

$$\epsilon_0 = E_0 - t_0, \tag{2.27}$$

where t_0 is the tunneling component. At sufficiently low T (large m^*), E_0 is accurately approximated by the lowest harmonic oscillator level:

$$E_0 = \tfrac{1}{2}m^{*-1/2} + O(T^2). \tag{2.28}$$

The splitting t_0 is given reasonably accurately by a standard WKB tunneling formula[25]:

$$t_0 = [E_0(T)/\pi]\exp[-I(T)], \tag{2.29}$$

where

$$I(T) = (2m^*)^{1/2}\int_{\phi_1+\delta\phi_1(T)}^{\phi_2-\delta\phi_2(T)} d\phi\,|E_0 - V(\phi)|^{1/2}. \tag{2.30}$$

The quantities $\delta\phi_1(T)$ and $\delta\phi_2(T)$ determine the temperature-dependent "turning points" for the WKB integral. Familiar limitations of WKB mean that the prefactor in (2.29) is only approximate[26,27] but important parameter dependences are reproduced as we shall see. For detailed numerical comparisons,[15] ϵ_0 should be taken from a direct numerical solution of Eq. (2.23).

Periodic potentials (e.g., SG) differ from unbounded ones in several respects. The transfer operator technique is still available, but the pseudo-Schrödinger equation (2.23) now poses a one-dimensional band-structure problem. If $V(\phi+\lambda)=V(\phi)$, then, in a reduced-zone scheme, we can label the eigenvalues $\epsilon_{n,k}$ with a band index n ($=0,1,2,\ldots$) and a wave vector k in the first Brillouin zone ($-\pi/\lambda < k \leq \pi/\lambda$). By Floquet's theorem the corresponding eigenfunctions have Bloch form:

$$\psi_{n,k}(\phi) = \exp(ik\phi) u_{n,k}(\phi), \tag{2.31}$$

with

$$u_{n,k}(\phi + \lambda) = u_{n,k}(\phi). \tag{2.32}$$

The tunnel-split levels in the case of two wells (Fig. 1) now form the extremities of a sequence of continuous bands. The low-temperature regime ($\beta E_K^{(0)} \gg 1$) corresponds to a tight-binding (narrow-band) limit, where the periodic functions $\{u_{n,k}\}$ are almost k independent and increasingly localized (in each well) as $T \to 0$. (At high T a free-electron picture is more appropriate.) For periodic potentials the lowest eigenvalue is not separated from from its neighboring excited states by a *finite* amount, so that Eq. (2.19) does not follow trivially as it does for any potential with a finite number of wells. However, a slightly more refined argument shows that (2.19) still applies.

In the case of the SG equation the eigenproblem (2.23) reduces to an analysis of the Mathieu equation which is extensively documented.[26,28] (For other periodic cases a more general Hill equation is involved.) For SG we can rewrite Eq. (2.23) in standard Mathieu form as

$$\left(\frac{d^2}{dz^2} + a - 2q\cos 2z\right)\psi(z) = 0 \tag{2.33}$$

with

$$z = \tfrac{1}{2}\phi, \quad a = 8m^*(\epsilon - 1), \quad q = -4m^*. \tag{2.34}$$

Reciprocal-lattice vectors are integers, since $\lambda = 2\pi$ for SG. The (characteristic) Mathieu functions at the zone center ($k = 0$) are periodic in ϕ with period 2π, while those at the zone boundary ($k = \frac{1}{2}$) are 4π periodic. These solutions are either even or odd.

The kink (soliton) rest energy [see Eqs. (2.7–2.9) and Table I] enters m^* [Eq. (2.25)] as

$$m^* = (\tfrac{1}{8}\beta E_K^{(0)})^2, \quad |q| = (\tfrac{1}{4}\beta E_K^{(0)})^2. \tag{2.35}$$

Asymptotic expansions for the position and width of each band at low T are available.[28] The center of each band is given by

$$\bar{\epsilon}_n \cong \frac{1}{8m^*}\left[2(2n+1)|q|^{1/2} - \tfrac{1}{8}[1 + (2n+1)^2] - \frac{(2n+1)^2}{2^7|q|^{1/2}}\left(2n+1+\frac{3}{2n+1}\right) - \cdots\right] \tag{2.36}$$

$$(n = 0, 1, 2, \ldots),$$

which becomes

$$\bar{\epsilon}_n \cong 4(2n+1)(\beta E_K^{(0)})^{-1} - [(2n+1)^2 + 1](\beta E_K^{(0)})^{-2} - \tfrac{1}{4}(2n+1)[(2n+1)^2 + 3](\beta E_K^{(0)})^{-3} - \cdots \tag{2.37}$$

$$(n = 0, 1, 2, \ldots).$$

The terms linear in T are simply harmonic-oscillator levels [c.f. (2.28)] for the sine-Gordon potential expanded to quadratic order about a single minimum. Eigenvalues in the nth band differ by exponentially small (tunnel-split) factors at low T. According to the improved WKB calculation by Goldstein,[26] the bandwidths are given to leading order by $2t_n(T)$, where

$$2t_n \cong \frac{2^{4(n+1)}}{n!}\left(\frac{2}{\pi}\right)^{1/2}(\tfrac{1}{4}\beta E_K^{(0)})^{n-1/2}\exp(-\beta E_K^{(0)}). \tag{2.38}$$

Contrast this behavior with that for the band gaps:

$$\bar{\epsilon}_{n+1} - \bar{\epsilon}_n \cong 8(\beta E_K^{(0)})^{-1} + O(T^2). \tag{2.39}$$

Returning to our general problem (2.1) we would like to know whether the kink [Eq. (2.5)] and phonon [Eq. (2.10)] excitations appear as elementary modes in the formal statistical mechanics, and in particular to what extent the excitations may be treated as a composition of noninteracting gases. Following the qualitative suggestions of Krumhansl and Schrieffer[6] (KS) in the ϕ^4 example, it is not difficult to demonstrate that the component E_0 of ϵ_0, taken together with *all* of F_ϕ [from Eq. (2.15)] *and* F_{V_0}, corresponds exactly to the free-energy density F_0 of a set of one-dimensional classical *harmonic* phonons (2.10) calculated to $O(l/d)$ to be consistent with Eq. (2.24). It is also essential that the lattice-dispersion relation, Eq. (2.13), be used in order to be consistent with the transfer-operator technique which was performed for a lattice. We find

$$\begin{aligned} F_0 &= \frac{k_B T}{2\pi}\int_{-\pi/l}^{+\pi/l} dk \ln(\beta\hbar\omega_k) \\ &= l^{-1}k_B T(\ln(\hbar\omega_0\beta) + \ln\{\tfrac{1}{2}[1 + (1 + 4d^2/l^2)^{1/2}]\}) \\ &\xrightarrow[l\to 0]{} k_B T[l^{-1}\ln(\hbar\omega_0\beta d/l) + (2d)^{-1}] \\ &= A\omega_0^2 E_0 - k_B T L^{-1}\ln Z_\phi + A\omega_0^2 V_0. \end{aligned} \tag{2.40}$$

This appealing identification of E_0 leads naturally to the equally physical speculation[6] that the tunneling contribution t_0 corresponds to the free energy of a gas of independent kinks defined by Eqs. (2.4)-(2.9). To investigate this suggestion consider first the limit $T \to 0$ in Eq. (2.30). Since $m^* \to \infty$ and $\delta\phi_{1,2} \to 0$ we find

$$\begin{aligned} I(T) \xrightarrow[T\to 0]{} I(0) &= (2m^*)^{1/2}\int_{\phi_1}^{\phi_2} d\phi\,[V(\phi)]^{1/2} \\ &= \beta E_K^{(0)}, \end{aligned} \tag{2.41}$$

where we have used Eqs. (2.4) and (2.9). Thus the tunneling free-energy density F_t has the asymptotic form

$$F_t(T) \underset{T\to 0}{\longrightarrow} -A\omega_0^2 t_0(0) \propto k_B T d^{-1} \exp(-\beta E_K^{(0)}). \tag{2.42}$$

The coefficient of proportionality omitted from Eq. (2.42) depends on the actual potential $V(\phi)$ and the accuracy[27] of the WKB approximation (2.29). This result is equivalent to the KS result for the classical free energy of a one-dimensional gas of indistinguishable, independent, static particles of width $\sim 2d$ and rest energy $E_K^{(0)}$ with kink density

$$\eta_K \propto d^{-1} \exp(-\beta E_K^{(0)}). \tag{2.43}$$

The results expressed by Eqs. (2.40) and (2.42) represent a general theorem, and in the ϕ^4 case led KS to suggest a phenomenology of independent gases of kink and phonon excitations. This important suggestion does indeed reflect quite general and central features of the nonlinear systems described by Eqs. (2.1) and (2.2). In one dimension some kinks will always be demanded by entropy considerations[29]; however, corrections are necessary because of *interactions* between kinks and phonons (and other excitations generally) for which we have so far not accounted; superposition is *impossible* in a nonlinear system. Fortunately, for some rather special examples of kinks exhibiting reflectionless (Bargmann[30]) potentials, the interactions (at least at low T) are especially tractable and allow some substantial analytic progress and physical interpretation, as we demonstrate in the next section. Both SG and ϕ^4 examples fall within this special class, but it is important to emphasize that the physical utility of a configuration-space philosophy is no less useful and applicable in more general cases[15,31-33]. Indeed, for a simple example involving a double-quadratic potential well of the form[34,35] $V(\phi) = \frac{1}{2}(|\phi| - 1)^2$, the kink presents a *nonreflectionless* potential for the phonons which can nevertheless be treated[33] analytically using both the transfer-operator approach and the phenomenological ideal-gas approach.

Improvements on Eq. (2.42) are clearly necessary: To obtain that result we took the limit $T \to 0$, in which case the kink velocity certainly tends to zero but so does the kink (and phonon) density. Similarly, we observe from Eq. (2.40) that *all* of the dynamical free energy (F_ϕ) is apparently taken up by the phonon modes as $T \to 0$. We shall see in the next section that this is remedied by a subtle *free-energy sharing* process via kink-phonon interactions, but from the formal transfer-operator point of view the remedy is that, to be consistent with a harmonic description, we must calculate $\delta\phi_{1,2}(T)$ to the *same* (linear T) order as $E_0(T)$ in Eqs. (2.29) and (2.30). Clearly $I(T) < I(0)$ for all $T > 0$. Explicit calculation within the WKB approximation [Eq. (2.30)] to linear-phonon order gives for the SG, ϕ^4, and DQ examples:

$$F_t \cong -\eta A \omega_0^2 (\sqrt{e}/\pi)(\beta E_K^{(0)})^{-1/2} \exp(-\beta E_K^{(0)}), \tag{2.44a}$$

where $\eta(\mathrm{SG}) = 16\sqrt{2}$, $\eta(\phi^4) = 2\sqrt{2/3}$, $\eta(\mathrm{DQ}) = 1$. Note the identical functional forms—potential details only affect the numerical prefactors. In fact, further improvements on the WKB approximation correct Eq. (2.44a) by the same factor[24,26,27,36] of $(e/\pi)^{1/2}$ yielding

$$F_t = -\eta A \omega_0^2 \pi^{-1/2} (\beta E_K^{(0)})^{-1/2} \exp(-\beta E_K^{(0)}). \tag{2.44b}$$

The correction of Eq. (2.42) by Eqs. (2.44) can be viewed as a (downward) thermal renormalization of the kink energy (see also Sec. V), but to make a detailed comparison with our phenomenology of excitation gases we require knowledge of how the excitations interact. In the next section we give a discussion of these interactions and their role in the phenomenology.

III. KINK-PHONON INTERACTIONS AND IDEAL-GAS PHENOMENOLOGY

In the previous section the free-energy density obtained via the transfer operator technique contained several features which suggested that one might be able to view the system as a gas of phonons and kinks, as originally proposed by Krumhansl and Schrieffer[6] (KS) for the ϕ^4 problem. The phenomenology proposed by KS neglected *all* interactions between phonons and kinks and, as a consequence, some essential features of a more appealing phenomenology were missed. Considerable progress has since been made in understanding the nature of the previously neglected kink-phonon interactions, and we devote this section to a discussion of their role in the statistical mechanics of the system.

The key to manageable calculation of kink-phonon interactions lies in recognizing at low temperatures, $k_B T \ll E_K^{(0)}$, the kink density will be very low, and as a consequence, the behavior of small oscillations (phonons) of the field in regions *between* the kinks will be very similar to the behavior of such oscillations in the kink-free system as a whole. This observation prompted KS to neglect[6] kink-phonon interactions altogether. Nonetheless, the phonon waveforms are modified in the presence of kinks, and the first step is to analyze this behavior and the resulting modifica-

tion of the phonon density of states (and free energy). To this end, we consider a system with only *one* kink present and find the resulting change in the phonon density of states. Then for a low density of kinks we assert that the total change in the phonon density of states is given approximately by the sum of the changes caused by each kink independently. We may view the kink modification of phonon free energy as a kink self-energy correction. This view is quite appealing since it provides us with a general prescription for any kink-bearing system of the wide class described by Eq. (2.2).

The behavior of small oscillations (e.g., phonons) $\chi(x,t)$ in the presence of a single static kink $\phi_K^{(0)}(x)$ is determined by solutions to Eq. (2.3) of the form

$$\phi(x,t)=\phi_K^{(0)}(x)+\chi(x,t)\ . \tag{3.1}$$

Phonons in the presence of moving kinks can be obtained from those for a static kink by "boosting" to the kink-rest frame. Substitution of Eq. (3.1) in Eq. (2.3) and linearization in χ leads to the following equation for χ:

$$\ddot{\chi}-c_0^2\chi_{xx}+\omega_0^2V''(\phi_K^{(0)}(x))\chi=0\ , \tag{3.2}$$

where $V''=d^2V/d\phi^2$ and the static kink waveform $\phi_K^{(0)}(x)$ is obtained from Eq. (2.5) with $v=0$. Writing χ as

$$\chi(x,t)=f(x)e^{-i\omega t} \tag{3.3}$$

leads to the following eigenvalue equation:

$$-c_0^2f_{xx}+\omega_0^2V''(\phi_K^{(0)}(x))f=\omega^2f\ . \tag{3.4}$$

Owing to the localized nature of the kink waveform $\phi_K^{(0)}(x)$, the function $V''(\phi_K^{(0)}(x))$ varies only in the region near the kink center ($x=0$) to any appreciable extent and approaches unity far away from the kink center:

$$V''(\phi_K^{(0)}(x))\xrightarrow[|x|\to\infty]{}1\ . \tag{3.5}$$

Moreover, the function $V''(\phi_K^{(0)}(x))$ has a minimum at $x=0$ such that

$$V''(\phi_K^{(0)}(x=0))<0\ . \tag{3.6}$$

From these properties we see that there exists a close analogy between Eq. (3.4) and the Schrodinger equation for a particle moving in a one-dimensional potential well $\omega_0^2V''(\phi_K^{(0)}(x))$. The bound state(s) and scattering or continuum states for this potential are of *fundamental* importance, not only for the statistical mechanics investigated here but also for use in perturbation theories[20,37] involving kink response to external perturbations or forces, as well as quantization procedures for kink states[3,38,39]. Examples of the potential function $V''(\phi_K^{(0)}(x))$ for the ϕ^4, SG, and DQ cases are given in Table I. Equation (3.4) can be solved exactly for these three cases, but for the moment we focus on *general* features for any $V(\phi)$ in the broad class of kink-bearing potentials.

Since our general Hamiltonian (2.2) possesses translation invariance, the spectrum of small oscillations about a single kink must contain a zero-frequency ($\omega=0$) translation mode (Goldstone mode) that restores[40] the translation invariance broken by the introduction of a kink into the system. This means that Eq. (3.4) must *always* possess a bound-state solution with $\omega_{b,1}^2=0$ (and perhaps other bound states with $0<\omega^2<\omega_0^2$) and the corresponding bound-state wave function $f_{b,1}(x)$ will be proportional to the spatial derivative of $\phi_K^{(0)}(x)$:

$$f_{b,1}(x)\propto[\phi_K^{(0)}(x)]_x\ . \tag{3.7}$$

It is trivial to show that $[\phi_K^{(0)}(x)]_x$ always satisfies Eq. (3.4) with $\omega^2=0$ by considering the spatial derivative of Eq. (2.3) [with $\phi=\phi_K^{(0)}(x)$]:

$$-c_0^2[\phi_K^{(0)}(x)]_{xxx}+\omega_0^2\,V''(\phi_K^{(0)}(x))[\phi_K^{(0)}(x)]_x=0\ . \tag{3.8}$$

Comparison of Eq. (3.8) with Eq. (3.4) shows the $f_{b,1}(x)\propto[\phi_K^{(0)}(x)]_x$ with $\omega_b^2=0$ is indeed a solution. Multiplication of $[\phi_K^{(0)}(x)]_x$ by a small constant and substitution into Eq. (3.1) yields a kink which had been uniformly translated by a small amount (hence the term "translation mode"). The frequency of this small oscillation is zero since the energy of a kink depends only on its velocity not on its position.

In addition to the translation mode at $\omega^2=0$ there may exist additional bound-state solutions of Eq. (3.4) with nonzero frequencies (between 0 and ω_0). The solutions correspond to internal oscillation modes in which the kink waveform undergoes a harmonically varying shape change localized about the kink center. The ϕ^4 case provides an example of this kind; there exists[29] exactly one additional bound state with $\omega_{b,2}=(\sqrt{3}/2)\,\omega_0$. For a general kink-bearing system [Eq. (2.2)], we denote the bound-state eigenfrequencies by $\omega_{b,1}=0,\omega_{b,2},\omega_{b,3},\ldots,\omega_{b,N_b}$, where N_b is the total number of bound states. The lowest of these will of course be $\omega_{b,1}=0$ (the translation mode) since all other $\omega_{b,n}^2$ must be non-negative if the kink is stable against small oscillations. In Table I we have listed the bound-state eigenfunctions for ϕ^4, SG, and DQ potentials.

In addition to the bound-state solutions of Eq. (3.4), there exist continuum states (extended modes) which we label by a wave vector k. These

states have eigenvalues ω_k^2 given by

$$\omega_k^2 = \omega_0^2 + c_0^2 k^2 , \tag{3.9}$$

which is precisely the dispersion relation for phonons in the absence of kinks. Equation (3.9) follows from the fact that far away from the kink the potential $V''(\phi_K^{(0)}(x))$ approaches unity [Eq. (3.5)]. Although the precise form of $f_k(x)$ depends on the potential and can be quite complicated in the region of the kink, we know that very far away from the kink the eigenfunction $f_k(x)$ must approach the form of an unperturbed phonon or superposition of unperturbed phonons with $+k$ and $-k$. The most general asymptotic forms needed for our purposes are

$$f_k(x) \underset{x\to\pm\infty}{\longrightarrow} A_k\, e^{i[kx \pm (1/2)\Delta(k)]} + B_k e^{-i[kx \pm (1/2)\Delta(k)]} , \tag{3.10}$$

where $\Delta(k)$ may be regarded as a phase shift which of course depends on the particular potential at hand. This phase shift contains *all* of the information concerning kink-phonon interactions that we shall need to construct the phenomenological free-energy density.

For those special cases (e.g., ϕ^4 and SG) where the potential $V''(\phi_K^{(0)}(x))$ is reflectionless,[30] we may choose B_k to be zero in Eq. (3.10), and the constant A_k is then determined by normalization. For less exotic cases (e.g., DQ) where the potential *is* reflecting, it is convenient to choose $B_k = A_k$, as first pointed out by Trullinger and DeLeonardis.[33]

In order to make contact with the transfer-operator results of Sec. II we consider a large system of length L and impose periodic (Born–von Karman) boundary conditions on the continuum (phonon) states $f_k(x)$. This periodicity condition, together with Eq. (3.10), gives the following condition for the allowed wave vectors:

$$L k_n + \Delta(k_n) = 2\pi n \quad (n = 0, \pm 1, \pm 2, \ldots) . \tag{3.11}$$

Clearly, the phonon density of states is *changed* by the presence of a kink:

$$\rho(k) = \frac{dn}{dk} = \frac{L}{2\pi} + \frac{1}{2\pi}\frac{d\Delta(k)}{dk} , \tag{3.12}$$

whereas the unperturbed density of states $\rho_0(k)$ in the absence of kinks is $\rho_0(k) = L/2\pi$, so that the change is given by

$$\Delta\rho(k) = \rho(k) - \rho_0(k) = \frac{1}{2\pi}\frac{d\Delta(k)}{dk} . \tag{3.13}$$

According to the Friedel sum rule,[41] there can be no *net* change in the total number of states when the kink is introduced. Since the number of bound states is N_b, the total number of phonon states must be *decreased* by N_b; i.e.,

$$\mathrm{P}\int dk\, \Delta\rho(k) = -\frac{1}{\pi}\Delta(0+) = -N_b , \tag{3.14}$$

where P denotes the Cauchy principal value, and we have used the fact that $\lim_{k\to\infty}\Delta(k) = 0$. Note that Eq. (3.14) also follows from Levinson's theorem[42]:

$$\Delta(0+) = \pi N_b .$$

One way to view this decrease is that kink "traps" phonon states due to its very presence. The number of states which it traps is unaffected by its velocity [Eq. (3.13) can be "boosted" to the kink rest frame[43]] and this number (N_b) must be at least one (corresponding to the translation mode). Not only is the trapping of at least one phonon state *unavoidable*, it is *precisely* the mechanism by which the kink can divert two degrees of freedom for its *creation* and *translation motion*. If additional phonon states are trapped, these provide the necessary degrees of freedom for the internal oscillations of the kink corresponding to the additional bound states of Eq. (3.4). We have thus isolated the novel mechanism by which degrees of freedom (or free energy, etc.) are *shared* between modes of a *nonlinear system*.

We are now in a position to calculate the *change* ΔF in the phonon free-energy density due to the presence of a kink moving at very low velocity $v \ll c_0$ (there will be very few kinks traveling with high velocity when $k_B T \ll E_K^{(0)}$). The velocity of the kink may then be neglected to zeroth order. We have then from Eq. (2.40)

$$\Delta F = \frac{k_B T}{L}\,\mathrm{P}\int_{-\pi/l}^{\pi/l} dk\, \ln(\beta\hbar\omega_k)\, \Delta\rho(k) , \tag{3.15}$$

or using Eq. (2.13)

$$\Delta F = \frac{k_B T}{L}\ln(\beta\hbar\omega_0)\,\mathrm{P}\int_{-\pi/l}^{\pi/l} dk\, \Delta\rho(k) + \frac{k_B T}{L}\,\mathrm{P}\int_{-\pi/l}^{\pi/l} dk\, \Delta\rho(k)\ln \times \ln\left[1 + 4\left(\frac{d}{l}\right)^2 \sin^2\left(\frac{lk}{2}\right)\right] . \tag{3.16}$$

In the limit as $l \to 0$, this becomes

$$\Delta F = -\frac{k_B T}{L} N_b \ln(\beta\hbar\omega_0) + \frac{k_B T}{L}\frac{1}{2\pi}\int_{0+}^{\infty} dk\, \frac{d\Delta}{dk}\, \ln(1 + d^2 k^2) . \tag{3.17}$$

In writing Eqs. (3.14) and (3.17) we have made use of the fact that $d\Delta/dk$ has a singularity on the

real axis only at $k=0$, so that $P\int dk$ can be replaced by $2\int_{0+}^{\infty} dk$ if the integrand is even, and by zero if the integrand is odd. We shall interpret this change in the phonon free-energy density as a contribution to the self-energy density of the kink. This viewpoint is similar in spirit to that adopted by Dashen, Hasslacher, and Neveu[38,44] in their calculations of the quantum renormalization of the kink mass due to its effect on the zero-point energy of the vacuum.

Another contribution to the kink self-energy density will arise from the localized internal harmonic oscillations of the kink corresponding to any additional bound states of the kink potential $V''(\phi_K^{(0)}(x))$ described above. The total self-energy of the kink is thus given by

$$\Sigma_K(T) = L\Delta F(T) + k_B T \sum_{n=2}^{N_b} \ln(\beta\hbar\omega_{b,n}), \tag{3.18}$$

where $\{\omega_{b,n}\}$ are the frequencies of the internal oscillations. The second term in Eq. (3.18) is absent if there is only one bound state ($N_b=1$).

At low temperatures ($k_B T \ll E_K^{(0)}$) the kink density will be exponentially small [see Eq. (2.43)] and hence the average separation between kinks (and antikinks) will be quite large. In this situation we associate the full value of $\Sigma_K(T)$ with each kink (antikink). With the large average separation between kinks we neglect kink-kink interactions to an excellent approximation.

In this phenomenological framework we may develop the thermodynamic functions for a system of phonons, kinks, and antikinks using the grand partition function. We consider ensembles of phonons, N_K kinks, and $N_{\bar K}$ antikinks. Of course, the phonons are perturbed by the presence of kinks, and the grand partition function, Ξ, cannot be rigorously factored; however, the implication of the immediately preceding discussion is that to a significant degree, the phonon-kink interactions can be accommodated by the self-energy corrections $\Sigma_K(T)$. Thus, we approximate

$$\Xi = \Xi_p^0 \Xi_{K,\bar K}, \tag{3.19}$$

where Ξ_p^0 is the *free* phonon grand partition function (GPF),

$$\Xi_p^0 = e^{-\beta L F_0} \tag{3.20}$$

with F_0 given by Eq. (2.40); $\Xi_{K,\bar K}$ is the kink-antikink GPF.

In the general class of kink-bearing systems it is necessary to distinguish between those in which which sequencing of kinks and antikinks is or is not constrained for physical reasons. In the sine-Gordon case, where the ground state is multiply degenerate, any sequence of kinks or antikinks is physically admissable; in the ϕ^4 and DQ cases, there being only two degenerate ground states, it is necessary that kinks be followed by antikinks (and vice versa). It follows that

$$\Xi_{K,\bar K} = \Xi_K \Xi_{\bar K} \quad (\mathrm{SG}), \tag{3.21a}$$

$$\Xi_{K,\bar K} = \Xi_{K,\bar K}^{\mathrm{ordered}} \quad (\phi^4, \mathrm{DQ}). \tag{3.21b}$$

In the former case

$$\Xi_K = \sum_{N_K \neq 0}^{\infty} e^{\beta\mu_K N_K} Z_K(N_K), \tag{3.22a}$$

where

$$Z_K(N_K) = \frac{1}{h^{N_K} N_K!}\left(\int_0^L dq_K \int_{-\infty}^{+\infty} dp_K \exp\{-\beta[(p_K^2 c_0^2 + E_K^{(0)2})^{1/2} + \Sigma_K]\}\right)^{N_K} \tag{3.22b}$$

and a similar set of expressions applies to antikinks with $N_{\bar K}, \mu_{\bar K}$.

For the constrained sequences in (3.21b)

$$\Xi_{K,\bar K}^{\mathrm{ordered}} = \sum_{N=0}^{\infty} e^{\beta\mu_K N} Z_{K,\bar K}(N), \tag{3.23a}$$

where

$$Z_{K,\bar K}(N) = \frac{2}{h^N}\left(\int_0^L dq_1 \int_0^{q_1} dq_2 \cdots \int_0^{q_{N-1}} dq_N\right)\left(\int_{-\infty}^{+\infty} dp_K \exp\{-\beta[(p_K^2 c_0^2 + E_K^{(0)2})^{1/2} + \Sigma_K]\}\right)^N \tag{3.23b}$$

$$= \frac{2}{N!}\frac{L^N}{h^N}\left(\int_{-\infty}^{+\infty} dp_K \exp\{-\beta[(p_K^2 c_0^2 + E_K^{(0)2})^{1/2} + \Sigma_K]\}\right)^N. \tag{3.23c}$$

Here N is the total number of kinks and antikinks ($N \simeq 2N_K$ in the limit of a large system); the multiplicative factor of 2 derives from the fact that sequences may start with either kink or antikink.

In the general sine-Gordon case, one may admit sequences for which $N_K \neq N_{\bar K}$, and their difference

$W = N_K - N_{\bar{K}}$ (called a winding number) has physical significance.[12,13] However, for systems with no externally applied bias toward kinks over antikinks, we expect $N_K = N_{\bar{K}}$ on the average, and $\mu_K = \mu_{\bar{K}}$. Restricting consideration here to that situation we find from Eqs. (3.22) and (3.23)

$$\Xi_{K,\bar{K}} = \exp[(2L/Bh)\alpha e^{\beta\mu_K}], \tag{3.24a}$$

where $B = 1$ (SG), $B = 2$ (ϕ^4, DQ). The quantity α results from the integration over p_K; it is expressible in terms of the modified Bessel function $K_1(\beta E_K^{(0)})$. Asymptotically, for large (βE_K^0)

$$\alpha = \frac{E_K^{(0)}}{c_0}\left(\frac{2\pi}{\beta E_K^{(0)}}\right)^{1/2} \exp[-\beta(E_K^{(0)} + \Sigma_K)]. \tag{3.24b}$$

When working in the low-density limit, except for the sequencing restriction taken care of numerically by the quantity B above, the kinks and antikinks may locate freely along the chain and we may choose to regard them as independent so that $\Xi_{K,\bar{K}} \simeq \Xi_K \Xi_{\bar{K}}$ where

$$\Xi_K = \Xi_{\bar{K}} = \exp[(L/Bh)\alpha e^{\beta\mu_K}]. \tag{3.24c}$$

The grand canonical potential density Ω is given by

$$\Omega = -(k_B T/L)\ln\Xi, \tag{3.25}$$

or, using Eqs. (3.19) and (3.24)

$$\Omega = F_0 - k_B T \frac{2E_K^{(0)}}{Bhc_0}\left(\frac{2\pi}{\beta E_K^{(0)}}\right)^{1/2} e^{\beta\mu_K} e^{-\beta(E_K^{(0)} + \Sigma_K)}. \tag{3.26}$$

The average total kink-number density $n_K^{\rm tot} = (N_K + N_{\bar{K}})/L = N_K^{\rm tot}/L$ is then given by

$$n_K^{\rm tot} = -\left(\frac{\partial\,\Omega}{\partial\mu_K}\right)_{T,L}. \tag{3.27}$$

We shall set the kink chemical potential μ_K equal to zero, since there is no external constraint on the kink number; the average kink density is then determined solely by the temperature. We set $\mu_K = 0$ after performing the derivative in (3.21) to obtain

$$n_K^{\rm tot} = \frac{2E_K^{(0)}}{Bhc_0}\left(\frac{2\pi}{\beta E_K^{(0)}}\right)^{1/2} e^{-\beta(E_K^{(0)} + \Sigma_K)}. \tag{3.28}$$

The free-energy density is given by $F = \Omega$ (with $\mu_K = 0$) or

$$F = F_0 - k_B T n_K^{\rm tot}. \tag{3.29}$$

The temperature dependence of $n_K^{\rm tot}$ can be explicitly displayed by combining Eqs. (3.17) and (3.18) to rewrite $\Sigma_K(T)$:

$$\begin{aligned}\Sigma_K(T) &= -k_B T N_b \ln(\beta\hbar\omega_0) + k_B T \frac{1}{2\pi}\int_{0+}^{\infty} dk \left(\frac{d\Delta}{dk}\right)\ln(1 + d^2k^2) + k_B T \sum_{n=2}^{N_b} \ln(\beta\hbar\omega_{b,n}) \\ &= -k_B T \ln(\beta\hbar\omega_0) - k_B T \sum_{n=2}^{N_b} \ln\left(\frac{\omega_0}{\omega_{b,n}}\right) + k_B T \frac{1}{2\pi}\int_{0+}^{\infty} dk \left(\frac{d\Delta}{dk}\right)\ln(1 + d^2k^2),\end{aligned} \tag{3.30}$$

where we have used the fact that $N_b \gg 1$ to isolate the first term in Eq. (3.30) and combine the remaining $-k_B T(N_b - 1)\ln(\beta\hbar\omega_0)$ with the sum over n. The temperature dependence of Σ_K is thus quite simple and motivates the following separation:

$$\Sigma_K(T) = -k_B T \ln(\beta\hbar\omega_0) - k_B T\sigma, \tag{3.31}$$

where the temperature-independent quantity σ is defined by

$$\sigma \equiv \sum_{n=2}^{N_b} \ln\left(\frac{\omega_0}{\omega_{b,n}}\right) - \frac{1}{2\pi}\int_{0+}^{\infty} dk\, \frac{d\Delta}{dk}\ln(1 + d^2k^2). \tag{3.32}$$

We note that since $\Delta(k)$ is a decreasing function of k and $\omega_{b,n} < \omega_0$, the quantity σ is positive. Equation (3.28) for $n_K^{\rm tot}$ may now be rewritten as

$$n_K^{\rm tot} = (2\pi)^{-1/2}(2e^{\sigma}/Bd)(\beta E_K^{(0)})^{1/2} e^{-\beta E_K^{(0)}}, \tag{3.33}$$

where we have used $d = c_0/\omega_0$. We emphasize that the *only* temperature dependence appearing in $n_K^{\rm tot}$ occurs through the ratio $E_K^{(0)}/k_B T = \beta E_K^{(0)}$. The temperature dependence of $n_K^{\rm tot}$ is therefore the *same* for *all* kink-bearing systems in our general class.

Using Eqs. (3.29) and (3.33) and the values of B and σ from Table I, we see that the kink free-energy density ($-k_B T n_K^{\rm tot}$) agrees *exactly* with the tunneling free-energy densities [Eq. (2.44b)]. Now that we have determined the free-energy density F given by Eqs. (3.29), (3.33), and (2.40), the other thermodynamic functions can be readily obtained. For example, the internal energy density $u = U/L = \partial(\beta F)/\partial\beta$ becomes

$$u = l^{-1}k_B T + (E_K^{(0)} - \tfrac{1}{2}k_B T)n_K^{\rm tot}. \tag{3.34}$$

This can be rewritten in the more suggestive form

$$u=(l^{-1}-N_b n_K^{\rm tot})k_BT + n_K^{\rm tot}[E_K^{(0)}+\tfrac{1}{2}k_BT+(N_b-1)k_BT], \quad (3.35)$$

or

$$U=Lu=(L/l-N_bN_K^{\rm tot})k_BT + N_K^{\rm tot}[E_K^{(0)}+\tfrac{1}{2}k_BT+(N_b-1)k_BT)]. \quad (3.36)$$

This is simply the internal energy of a system with $(L/l-N_bN_K^{\rm tot})$ classical phonon modes and $N_K^{\rm tot}$ nonrelativistic particles of rest energy $E_K^{(0)}$ each having $\frac{1}{2}k_BT$ translational energy and thermal energy (k_BT) for each of the N_b-1 internal oscillation modes. Thus, the kinks obtain their necessary degrees of freedom at the expense of precisely the correct number of degrees of freedom in the phonon modes. The entropy S is easily found to have the form

$$\frac{S}{k_B}=\frac{L}{l}\left[1-\frac{l}{2d}-\ln\left(\beta\hbar\omega_0\frac{d}{l}\right)\right] + N_K^{\rm tot}\left(\frac{E_K^{(0)}}{k_BT}+\frac{1}{2}\right), \quad (3.37)$$

and the specific heat $c_L=(\partial u/\partial T)_L$ has the form

$$c_L=k_Bl^{-1}+k_B\{[(E_K^{(0)}/k_BT)-\tfrac{1}{2}]^2-\tfrac{1}{2}\}n_K^{\rm tot}. \quad (3.38)$$

All of the thermodynamic functions (F,u,S,c_L) are, of course, dominated by phonon contributions, since the kink density is exponentially small at low temperatures $(\beta E_K^{(0)}\gg 1)$. However, the density of kinks is quite important information for several features which are insensitive to phonons; for example, the dc conductivity in charge-density-wave condensates[9] and certain correlation functions for the field as discussed in Sec. V.

We conclude this section with some remarks concerning higher T orders in the functional integral result for the free-energy density. For integrable systems such as SG (see Sec. IV) a formally analytic configurational phenomenology is still possible. In other cases (including ϕ^4 and DQ) it is not, and a phenomenological picture has to be approximate. Nevertheless, such a picture can still be remarkably successful even at $k_BT\simeq E_K^{(0)}$ and is a very pertinent conceptual device even though approximate schemes to renormalize the kink energy must be used.[45,46] In general two new features appear in the exact transfer-operator expressions at higher T. First, a polynomial series[28] in $(k_BT/E_K^{(0)})^{1/2}$ replaces the simple prefactor in Eqs. (2.44). This is expected because the second change is that $E_0(T)$ develops a power-series form as shown for example in Eq. (2.37) for SG. Similarly, deviations from the tight-binding band structure develop for cases where $V(\phi)$ is periodic (e.g., SG). It is clear that these correspond to anharmonic kink-phonon effects. Note from Eq. (2.37) that the free energy is lowered by the negative anharmonicity consistent with general theorems.[47] *Rigorous* phenomenology (certainly in nonintegrable systems) will be difficult; these new terms have to account for (virial) kink-kink corrections, as well as interactions with anharmonic phonons and other excitations appearing beyond linear order.[48-49] Interactions between modes have been little-explored in these regimes. The corrections to $E_0(T)$ itself have nothing to do with kinks (which are related to exponential tunneling factors).

In this section we have seen that kink and phonon excitations give rise to characteristic contributions to the equilibrium thermodynamic functions for a *general* class of nonlinear Hamiltonians [Eqs. (2.1) and (2.2)]. Detailed interpretation even at low T, however, was found to require knowledge of *interactions* between these excitations. This knowledge was shown to reside in the phase-shift function $\Delta(k)$ which was found to have a particularly simple form for the three example cases presented (ϕ^4, SG, DQ). We have shown that the low-temperature statistical mechanics can be interpreted in terms of mode conservation and energy-sharing mechanisms and that the low-temperature ideal-gas phenomenology is exact.

In the following section we discuss the sine-Gordon case in particular since it provides an example of a completely integrable system for which the above phenomenology should, in principle, be extendable to *all* orders of nonlinearity by inclusion of breather excitations.

IV. SINE-GORDON AS AN INTEGRABLE HAMILTONIAN SYSTEM: THE BREATHER PROBLEM

In principle, totally integrable Hamiltonian systems, such as the continuum SG, are ideally suited to an *exact* phenomenological formulation of classical statistical mechanics. The concepts of partitioning solution space into nonlinear normal modes and energy-sharing (developed to *linear* order in Sec. III) generalize exactly. This is because *exact* soliton equations are (with some restrictions on boundary conditions) completely soluble via (for example) the inverse scattering transform,[2,50-52] a *canonical* transform to functions of generalized action-angle variables which serve to label allowed types of elementary excitations. Among other remarkable properties the allowed excitations are infinitely long-lived, suffering purely asymptotic pair-wise additive phase shifts and forming normal modes in the sense (for instance) that the Hamiltonian is exactly separable into contributions from each

constituent mode. These properties will be recognized as nontrivial generalizations of those used in Sec. III, which were only valid in a low-density regime. The same separability extends to quantized integrable Hamiltonian systems; eigenstates appear[53] as solutions derivable from a generalized Bethe ansatz[54] and all collisions are elastic and preserve momentum, so that the S matrix is exactly factorable. In the case of SG, the nonlinear normal modes are solitons (and antisolitons), continuum excitations, and breathers. Only the first two of these mode types were needed in the low-T theory of Sec. III.

Complete details of action-angle variables for SG can be found in Refs. 14, 51, and 52 with necessary phase-shift results in Refs. 14 and 43. We have chosen not to reproduce these here because fundamental obstacles to the inclusion of breather modes in a classical statistical-mechanics calculation remain and we will postpone detailed discussion to a succeeding publication except for the following brief remarks.

The single SG breather translating at velocity v ($v < c_0$) (see Sec. II for notation) has the form

$$\phi_B(x,t;v,\omega_B) = 4\tan^{-1}\left(\frac{(\omega_0^2/\omega_B^2-1)^{1/2}\sin[\gamma\omega_B(t-vx/c_0^2]}{\cosh[\gamma d^{-1}(x-vt)(1-\omega_B^2/\omega_0^2)^{1/2}]}\right) \tag{4.1}$$

with energy

$$E_B(v,\omega_B) = 2\gamma E_K^{(0)}\,(1-\omega_B^2/\omega_0^2)^{1/2}\,. \tag{4.2}$$

Here, $E_K^{(0)}$ is the SG kink rest energy given in Table I, ω_B ($0<\omega_B<\omega_0$) is the frequency with which the breather envelope oscillates harmonically (in its center-of-mass frame), and we have omitted two phases representing conjugate variables to the translational and internal momenta. Note that as $\omega_B \to 0$, the breather amplitude approaches 2π, its width approaches twice the soliton width, and it unbinds to become a soliton-antisoliton pair. On the other hand as $\omega_B \to \omega_0$ the breather profile becomes very extended and of low amplitude. As might be expected from these limits, breathers can be viewed either as soliton-antisoliton bound states or as anharmonic phonons.[38] Indeed, upon quantization,[14,38] breathers appear naturally as multiphonon bound states and the lowest-energy breather coincides with the fundamental quantized mode (phonon) in all physical properties. Nevertheless, classically, the breather does not become a linearized phonon as $\omega_B \to \omega_0$, since its frequency must be less than ω_0 and its amplitude still depends on its frequency.

Breathers are of interest in several physical contexts[5,8,9,38,39] because they combine internal dynamic structure with a particlelike envelope. In particular, their contributions to thermodynamic quantities need to be considered at all but the lowest temperatures where linear phonons are sufficient (Sec. III). Certainly breather excitations are observed in molecular dynamics simulations of sine-Gordon[55] and ϕ^4 (Ref. 56) chains, although they do not enjoy the topological stability of kink solitons and are more sensitive to discrete lattice effects.

Since breathers do not break global symmetry, anharmonic-phonon perturbation theories or mode-mode coupling theories of suitable finite order for equilibrium or nonequilibrium statistical mechanics accurately include low-amplitude breather contributions. However, these will not emphasize the distinctive spatial and temporal *coherence* characterizing breathers. This can be important, especially when shorter breathers are substantially populated and for interpreting certain dynamic responses.[55] It is important to note that the several phenomenological approaches[57-69] to nonlinear statistical mechanics (as well as the transfer integral technique) which treat the dynamic and configurational partition function components separately can accommodate kinks naturally, since these appear as static steepest-descent trajectories in a path integral representation. Breathers or phonons are less natural. They require perturbation around steepest-descent trajectories and their internal dynamics means they must be reconstructed by a suitable recombination of dynamical and configurational components. The direct nonlinear normal-mode phenomenology available for integrable systems already includes such spatial *and* temporal ordering. This is why it is so physically appealing.

Many of these statements for breathers apply equally to all nontopological pulse solitons as in the nonlinear Schrödinger equation,[2] solitons of the Heisenberg ferromagnetic chain,[60] Korteweg–de Vries equation,[2] Toda lattice,[2] etc. Statistical mechanics in a soliton basis is intrinsically more difficult in these cases than for kink solitons. The latter have a finite creation energy so that there will always be a temperature (≈creation energy) below which the soliton density is exponentially low. Pulse solitons, however, have a range of creation energies extending to zero. We can then expect power-law temperature dependen-

cies in the free energy, soliton density, etc., rather than activated forms. In addition, mode counting will be more critical than for a dilute kink gas—arbitrarily low-energy pulse solitons can be populated with arbitrarily high density, so that discrete lattice and finite-size limits need to be handled carefully.

In the case of SG breathers, these concerns become clear if we use the inverse-scattering theory naively. Namely, as a generalization of the low-T kink approach (Sec. III), we can construct a grand canonical partition function for an ideal gas of renormalized breathers. The renormalization derives from pair-wise additive phase-shift interactions with phonons (as in Sec. III), which can be given exactly for integrable systems.[14,43] Each breather removes two phonon modes consistent with its interpretation as a soliton-antisoliton pair. Integrating over all breather velocities, internal frequencies, and conjugate variables it is possible[61] to evaluate a breather partition function to *all* orders in T. The corresponding free energy contains a power series in T as expected [c.f. the transfer integral expansion (Sec. II)] but also an explicitly *divergent* term. As anticipated, this divergence arises from the high-frequency ($\omega_B \to \omega_0$) breathers.

It is clear that the large number of breather modes expected even at low T directs attention to several points. These include the following: (i) The inverse-scattering theory which generates the separable Hamiltonian structure used in the above approach distinguishes *coincident* breathers or kinks, i.e., multiple numbers of these with the *same* momenta *and* conjugate (position) variables. Formally, solitons and breathers appear in inverse-scattering theory as poles and pairs of poles in the eigenvalue plane of an auxiliary linear operator. The usually quoted[50] separable form assumes only simple poles: Multiple poles and pairs of multiple poles must be treated specially. This area is little studied[62] and is omitted in the calculations of Sec. III and the above description. We cannot expect an important effect for kink contributions at low T because the kink density is activated and coincidences are of a much lower order. However, such coincidences will become important even at low T for breathers since arbitrarily low creation energies are possible classically. (ii) The possibilities of arbitrarily low-energy breathers and correspondingly high densities means that mode conservation must be included precisely. In particular, the order of thermodynamic limit and integration over breather variables has to be handled carefully—boundary effects for extended breathers are important. (Note that the most-studied inverse-scattering procedure assumes decaying boundary conditions.[50]) (iii) Since linear phonon modes are viewed quantum-mechanically as the low-energy part of the breather spectrum[14,38] we can expect that the classical statistical-mechanics limit will have to be defined carefully, particularly with regard to the *high*-frequency breathers. Recall that the classical limit was introduced explicitly in the transfer integral approach by the separation of dynamic and configurational free energy (Sec. II). Similarly, the kink-phonon phenomenology (Sec. III), included the classical criterion $k_B T \gg \hbar\omega_0$ in the harmonic phonon free-energy expression [cf., Eq. (2.40)]. We will return to the analysis of statistical mechanics for breather-like excitations in a separate publication.

V. CORRELATION FUNCTIONS

The concept of a configurational phenomenology is especially important in the analysis and interpretation of equilibrium static and dynamic correlation functions (as well as in certain transport coefficients[63]). The soliton solutions, in particular, manifest themselves as long-lived excitations (at low T) with novel physical consequences—for example, an intrinsic low-frequency response mode.[6] Although in principle the knowledge of the complete evolution available for totally integrable Hamiltonian systems (Sec. IV) allows $S(q,\omega)$ to be formulated in normal-mode basis, in practice this has been of limited value and little *analytic* improvement on bare phenomenology[6] has been made.[49,64-66] A complete survey of phenomenologies (in integrable and nonintegrable systems) for $S(q,\omega)$ and of experimental implications is beyond the scope of this work and will be given in a separate publication.[67] Here we will limit discussion to the *static* structure factor, i.e., the integrated intensity $\int d\omega\, S(q,\omega)$ or equivalently the equal-time correlation function [e.g., (2.20)] related by Fourier transform. In this limit an exact solution via the transfer integral technique is available against which phenomenologies can be calibrated.

Typical correlation function expressions from the transfer integral approach were given in Eqs. (2.20–2.22) (generalization to some very anisotropic higher-dimensional models is also possible[15]). In q space the equivalent results are, introducing the intermediate scattering function $F(q,t)$,

$$\int d\omega\, S(q,\omega) = F(q,0) = \int dx\, C_1(x) e^{iqx}$$

$$= \sum_n |\langle 0|\phi|n\rangle|^2 \frac{\lambda_n}{q^2\lambda_n^2+1} \quad , \tag{5.1}$$

where λ_n is a characteristic correlation length:

$$\lambda_n^{-1}(T) = \beta A \omega_0^2 (\epsilon_n - \epsilon_0) \ . \tag{5.2}$$

The distribution $F(q, 0)$, then, appears as a weighted sum of Lorentzians. (In this it is related to solutions of certain Fokker-Planck *nonequilibrium* distributions in a large damping regime, which can also be reduced to a pseudo-Schrödinger Hamiltonian problem.[68])

In many cases of interest it is possible to restrict the sum (5.1) considerably for $|x| \gg \lambda(T)$. Consider, for instance, a symmetric double-well potential $V(\phi)$ in (2.2) (e.g., the ϕ^4 model). We deduce from symmetry that the lowest level with nonzero-matrix element (i.e., coupling to the ground state $n=0$) is $n=1$, the first excited level. Then from (2.44b) and (5.2)

$$\lambda_1(T) \underset{T \to 0+}{\longrightarrow} (\tfrac{1}{24}\pi)^{1/2} \, d(\beta E_K^{(0)})^{-1/2} \exp(\beta E_K^{(0)}) \ , \tag{5.3}$$

where we have adopted the specific numerical coefficient for ϕ^4; the functional form of (5.3) is general. The exponential kink-energy dependence is characteristic of coupling between *tunnel-split* levels ($n=0, 1$). Higher-n-levels differ from $n=0$ essentially as different levels in a single-well potential and give a dominant power-law temperature dependence to the corresponding correlation lengths. Indeed, at low T we can approximate the levels with harmonic oscillator states (2.28): $\epsilon_n - \epsilon_0 \propto k_B T / E_K^{(0)}$. Thus

$$\lambda_{n \geq 2} \propto d(+ O(k_B T / E_K^{(0)}), \ O(e^{-E_K^{(0)}/k_B T})) \ . \tag{5.4}$$

In this situation $\lambda_1 \gg \lambda_{n \geq 2}$ so that (5.1) is well approximated (at large $|x|$) by

$$F(q, 0) \simeq |\langle 0 | \phi | 1 \rangle|^2 [\lambda_1 / (q^2 \lambda_1^2 + 1)] , \tag{5.5}$$

i.e.,

$$C_1(x) \simeq |\langle 0 | \phi | 1 \rangle|^2 \exp(- |x| / \lambda_1) \ . \tag{5.6}$$

The temperature dependence of the matrix elements is weak,[15,67] dominated at low T by phonon fluctuations: $|\langle 0 | \phi | n \rangle|^2 \sim 1 - \alpha_1 k_B T / E_K^{(0)}$ ($n=1$) and $\sim \alpha_n (k_B T / E_K^{(0)})^2$ ($n \geq 2$) (for n such that $\langle 0 | \phi | n \rangle \neq 0$) with α_n being numerical coefficients. Consequently, in examples of this type (i.e., coupling between tunnel-split levels) a characteristic kink activation appears *directly* in the correlation length. A simple phenomenological interpretation is then available at low T similar to that for pure one-dimensional Ising models.[15,45,46] We consider a gas of independent kinks in one-dimension with a Poisson separation distribution. Each kink has the property that its passage flips the field variable ϕ from $\pm \phi_0(T)$ to $\mp \phi_0(T)$ with $\phi_0(T) \to \phi_1$ (Fig. 1) as $T \to 0+$. Furthermore, the kink and antikink always follow each other. Introducing $N_K(x)$, the number of kinks in the interval x, it is easily shown that

$$\begin{aligned} C_1(x) &= \langle \phi(x) \phi(0) \rangle \simeq \phi_0^2(T) \, \langle (-1)^{N_K(x)} \rangle \\ &= \phi_0^2(T) e^{-|x| \lambda_K^{-1}} \end{aligned} \tag{5.7}$$

with

$$\lambda_K(T) = [2 \, \langle n_K^{\text{tot}}(T) \rangle]^{-1} \ . \tag{5.8}$$

In this phenomenology, phonon fluctuations are relegated (for large $|x|$) to $\phi_0(T)$ and the kink dressing implicit in $\langle n_K^{\text{tot}}(T) \rangle$ (Secs. II, and III). With the identification $\epsilon_1 - \epsilon_0 = (2/\beta A \omega_0^2) \langle n_K^{\text{tot}}(T) \rangle$ (Secs. II and III) and $\phi_0^2(T) = |\langle 0 | \phi | 1 \rangle|^2$, we see that (5.7) and (5.8) agree with the exact result (5.6).

This kind of strong signature for order-parameter defects in the correlations of strongly nonlinear systems is in fact quite general, extending to models on higher-dimensional lattices and with multi-component order parameters [recent examples have included the classical (isotropic and anisotropic) planar and Heisenberg models[32,69]]. However, there are other important situations where phenomenological interpretations are less transparent—for example, if we consider correlations of a function $\tilde{F}(\phi)$ which is unchanged after the passage of a kink, e.g., $\tilde{F} = \phi^{2n}$ (n integer), $|\phi|$, etc. (relevant to, e.g., energy-energy correlations). Clearly, correlations in these cases are dominated by the almost complete Bragg peak [with weight softened only by the phonons (Debye-Waller factor)] and an exponentially small volume occupied by kinks. Additional correlations only reflect the phonon and local-defect (kink) regions. Both of these are determined by the *short*-length scale d (~kink width) and *not* the average kink separation as in (5.8): The fluctuation correlation length does not diverge as $T \to 0+$ and does not reflect the kink activation energy. Kinks are nevertheless still a striking physical aspect of the *dynamics* and a phenomenology is still possible which incorporates them.[66,67]

In the *static* case, the differing properties of this last situation follow immediately from the transfer integral formalism. We simply note that $\langle 0 | \tilde{F}(\phi) | 0 \rangle \neq 0$, which in (5.1) gives us the Bragg peak. Expansions of $\langle 0 | \tilde{F} | 0 \rangle$ at low T then allow us to identify kink and phonon depletions of the Bragg amplitude.[67] By symmetry

$\langle 0|\tilde{F}|1\rangle \equiv 0$ so that the characteristic kink correlation length no longer appears and indeed all of the contributing terms in (5.1) have correlation lengths $\lambda_n(T)$ of the form (5.4). The corresponding matrix elements $|\langle 0|\tilde{F}|n\rangle|^2$ each contain phonon and kink terms.[67] In such cases, then, kink effects appear through the matrix elements and *not* the eigenstructure of the effective Schrödinger equation (2.23). In practice many terms must be kept in (5.1) to reproduce the kink and phonon effects adequately. Phenomenology is therefore even more appealing.

It will appreciated that the q and T dependence of $F(q, 0)$ are quite different for the two types of situations described above. Compare, for instance, the different ways in which the eventual complete Bragg peak evolves as $T \to 0+$.

Essentially the same questions arise when we consider examples of (2.2) with periodic $V(\phi)$ such as SG. Here the appropriate order parameter or physically interesting variable frequently arises as a *periodic* function $F_p(\phi)$ of the field; ϕ might be a phase,[9] spin rotation,[66] etc. In view of the Floquet structure of the eigenfunctions of the effective Schrödinger Hamiltonian (2.23), matrix elements of periodic functions are severely restricted. Matrix elements of nonperiodic functions of ϕ do arise in the analysis of mass (charge, spin, etc.) diffusion and transport described by SG-like models.[63] These have very different properties and consequences not available in unbounded potentials—the possibility of mass diffusion distinguishes periodic potentials $V(\phi)$. We will describe here correlations only of periodic forms F_p which are of greatest interest in scattering experiments, etc.

The two types of behavior we experienced for ϕ^4 both occur, depending on the specific form of $F_p(\phi)$ and the relative periodicity of $F_p(\phi)$ and $V(\phi)$. For definiteness we choose $F_p(\phi)$ to be 2π-periodic and freely oscillating [$F_p(\phi) = e^{i\phi}$, $\cos\phi$, etc.] as is most usual. Then, if $V(\phi)$ has periodicity 2π, a kink does not change the asymptotic value of F_p and we anticipate analogous behavior to ϕ^2 correlations in the ϕ^4 model. The only characteristic length is again the kink width d. On the other hand if $V(\phi)$ is $(2\pi/N)$ periodic ($N \geq 2$, integer), the analogy with ϕ correlations in an N-well model can be expected. [Lower-symmetry cases (periods $2\pi N$) will not differ qualitatively from the 2π-periodic case.]

These physical expectations again appear naturally within the transfer integral formalism. Consider the correlation function $C_{\text{periodic}}(x)$, (2.22). (Other choices are entirely parallel.) Adopting the Bloch function form (2.31) we have now to consider matrix elements of the type

$$\langle 0|e^{i\phi}|k\rangle \equiv \int_{-\infty}^{+\infty} d\phi\, u_0(\phi) u_k(\phi)\, e^{i(k+1)\phi}, \qquad (5.9)$$

where $u_k(\phi) = u_k(\phi + \xi)$ with $\xi = 2\pi/N$. Here we have adopted the extended zone scheme for pedagogic convenience ($-\infty < k < \infty$). Despite the continuous (band-structure) eigenspectrum, the periodicity of all functions in (5.9) demands the selection rule (Bragg condition)

$$k + 1 = G\,, \qquad (5.10)$$

where G is a reciprocal-lattice vector, $G = 2m\pi/\xi$ (m integer). If $\xi = 2\pi$, then (5.10) shows that the ground state $k = 0$ is coupled to states $k = 0, \pm 1, \pm 2, \ldots$, i.e., only to $k = 0$ states of each band in the reduced-zone scheme (2.31). The self-coupling of the ground state simply provides the Bragg peak as in the ϕ^4 case for ϕ^2 correlations: $|\langle 0|e^{i\phi}|0\rangle|^2 = 1$ (– phonon and kink pieces, omitting a trivial normalization factor). Fluctuations with respect to this average arise from the excited $k = 0$ states, which are all separated from the ground state by band *gaps*. At low T these $\sim k_B T/E_K^{(0)}$ [(c.f. (2.39)]: Tunnel-splitting corrections are exponentially small, exactly as in ϕ^4. From (2.38) we see that the correlation lengths (5.2) for the SG example are $\lambda_n \to nd$, as $T \to 0+$. Again the fluctuations (with respect to the ground-state average) remain short-ranged as $T \to 0+$, and the only kink signatures arise in the matrix elements as depletions of the Bragg peak or fluctuations amplitudes. It is necessary to consider the dynamic response $S(q, \omega)$ for a strong kink characteristic (low-frequency mode) to appear.[66,67]

Contrast the periodicity $\xi = 2\pi$ with $\xi = 2\pi/N$ ($N = 2, 3, \ldots$). Now the Brillouin zones are stretched, $G = mN$, and from (5.10) we conclude that coupling exists between the ground state and the excited state in the first band at $k = (-2/N) \times$ (zone boundary wave vector, $\frac{1}{2}N$). These states are separated by tunnel-splitting and therefore dominate the sum (5.1) (for large $|x|$), directly reflecting the kink activation energy. In particular for $N = 2$, coupling is to the top of the first band and from (2.38) for the SG case

$$\lambda^{(N=2)}(T) \simeq \tfrac{1}{8} d (\tfrac{1}{2}\pi)^{1/2} (\beta E_K^{(N=2)})^{-1/2} \times \exp(E_K^{(N=2)}/k_B T). \qquad (5.11)$$

The Ising-model picture (5.7) and (5.8) then applies immediately. For $N > 2$ coupling to a lower state in the first band is allowed. Using a tight-binding band structure (appropriate at low T) we find explicitly that [for a general $V(\phi)$ of this periodicity]

$$\lambda^{(N)}(T) \simeq \frac{2\lambda^{(N=2)}\,(E_K^{(N=2)} - E_K^{(N)} = 2E_K^{(N=2)}/N)}{1-\cos(2\pi/N)} . \tag{5.12}$$

The divergence of the correlation length as $T \to 0+$ with kink activation is therefore still dominant; the phenomenological analogy is now with a higher spin model. In all cases $N \geq 2$, $\langle 0|e^{i\phi}|0\rangle \equiv 0$ in accord with our physical expectation that long-range correlations in $e^{i\phi}$ are destroyed by kinks in these cases. Note from (5.12) that at sufficiently low T, $\lambda^{(N>2)}(T) < \lambda^{(N=2)}(T)$: Physically, each kink changes $e^{i\phi}$ by a smaller amount for $N>2$ but the kink density is greater and dominates.

It may be useful to visualize the results of this section by considering our periodic $V(\phi)$ models as a classical one-dimensional XY fixed-spin model in an N-fold anisotropy field (e.g., $\propto [1-\cos(N\phi)]$): $S_X^i S_X^{i+1} + S_Y^i S_Y^{i+1} - S^2\cos(\phi_{i+1}-\phi_i) \simeq S^2(d\phi/dx)^2$; $S_x = S\cos\phi$, $S_y = S\sin\phi$. If $N=1$, the anisotropy term is equivalent to an applied field and $\phi(x)=0$ is the nondegenerate ground state (c.f., $<0|e^{i\phi}|0>\neq 0$ for $N=1$). With $N \geq 2$, however, there are physically distinct minima for ϕ in $(0, 2\pi)$—the ground state is degenerate (c.f., $\langle e^{i\phi}\rangle = 0$, $N \geq 2$). Kinks describe spin rotations evolving between neighboring minima. Thus, we again expect 2π-periodicity ($N=1$) to be qualitatively distinct. Note also from (5.12) that as the degree N of the anisotropy $\to \infty$, $\lambda^{(N)} \to \infty$, and the symmetry-breaking becomes irrelevant. This behavior is also evident in treatments of the anisotropic two-dimensional classical XY model.[32]

The spin example above is actually of current experimental interest for the special case $N=1$—$CsNiF_3$ (for example) in an applied magnetic field is a planar ferromagnet quite well described by the model[66] and evidence of soliton dynamics in $S(q,\omega)$ has been reported.[70] Other physical realizations of the periodic $V(\phi)$ models include spin, phonon, and electronic systems experiencing a commensurability potential.[71] In fact, periodicities of fractional order ($\xi = 2\pi M/N$; M, N integers) can then be relevant but the discussion of correlations given above is readily generalized. A recent numerical analysis[16] of a similar model with twofold symmetry breaking ($\xi = \pi$) but including amplitude fluctuations in a complex order parameter $\psi = |\psi|e^{i\phi}$ has established similar kink signatures in appropriate correlations, and a recent analytic investigation[72] of this model had confirmed the presence of two-component kink excitations.

VI. SUMMARY AND DISCUSSION

In this paper we have extended the ideal-gas phenomenology of Krumhansl and Schrieffer[6] to include the entire class of nonlinear Klein-Gordon models [Eq. (2.3)] having topological kink solutions in one dimension. By taking into account the phonon phase shifts which occur in the presence of kinks, we have isolated the mechanism for sharing of energy and degrees of freedom among the elementary excitations of the nonlinear system. We have shown that this configuration or nonlinear normal-mode phenomenology gives the exact low-temperature behavior of the various thermodynamic functions and correlation lengths by comparing the phenomenological results to those obtained via the exact transfer operator technique. Thus, by properly incorporating kink self-energies due to reduction of the phonon density of states in the presence of kinks, we have placed KS theory on a firm foundation. We have found that the low-temperature density of kinks is given by a universal temperature dependence $n_K \sim (\beta E_K^{(0)})^{1/2}\exp(-\beta E_K^{(0)})$, where only numerical prefactors are model dependent and the temperature enters only through the ratio $\beta E_K^{(0)} = E_K^{(0)}/k_B T$. The usefulness of the phenomenology is now apparent since one need not carry out a calculation of the partition function for each case of interest, but only a calculation of the kink rest energy $E_K^{(0)}$ via Eq. (2.9).

We conclude by mentioning a few extensions of the phenomenology which are currently under investigation. While we have focused in this paper on one-component fields, there may be several situations where multi-component fields need to be considered.[72-74] For example, in solitary-wave-bearing charge-density-wave systems,[9] the amplitude as well as the phase of the condensate carries degrees of freedom so that, in general, the field has *two* components. Evidence for two-component solitary waves in the statistical mechanics of such systems has already been found[16] numerically via the transfer operator approach and also via a recent analytic treatment.[72] However, it remains to develop an ideal-gas phenomenology analogous to that developed here for one-component models. The same physical ideas should be applicable to the two-component problem where both phase and amplitude-phonon densities of states will be affected by the presence of kinks, and an investigation is currently in progress.[73]

In this paper we have considered only the *classical* statistical mechanics of one-component solitary-wave-bearing fields. However, it is clear that quantum corrections may become important at low temperatures. Indeed, it has recently been shown[39] that the thermal density of quantum SG solitons varies as $n \sim (\beta E_K^{(0)})^{-1/2} \times \exp(-\beta E_K^{(0)})$ which differs from the classical density in the exponent of the prefactor. This difference

arises because[39] of zero-point renormalization of the kink energy rather than the thermal phonon renormalization considered here. The quantum phenomenology[39] also needs to be extended to multicomponent fields.

Another area of extension is to nonequilibrium situations such as occur when the system is placed in an external field and damping mechanisms are included. A recent calculation[63] of the nonlinear response of the SG chain has been carried out via the Fokker-Planck approach. In the low-temperature, low-field limit, the response is dominated by thermalized solitons. However, at higher fields the role of solitons has not yet been explicitly identified in the exact results, although recent molecular-dynamics simulations[75] clearly show the existence of kink excitations. A nonequilibrium kink phenomenology is clearly desirable and some efforts in this direction have been made.[76]

Finally, in order to extend the phenomenology to higher temperatures, we still need to determine how the breatherlike excitations (Sec. IV) enter the statistical mechanics; in addition, as the kink density is increased by raising the temperature, we expect virial corrections to become important. An investigation of the virial expansion is currently underway.[77]

Note added in proof. Very recently, DeLeonardis and Trullinger (unpublished) have used the analytic properties of the phase-shift function, $\Delta(k)$, to obtain a closed form expression for the kink self energy [Eqs. (3.31) and (3.32)] valid for the entire class of kink-bearing potentials $V(\phi)$ considered here. In addition to explicitly demonstrating the low-temperature exactness of the ideal-gas phenomenology for all $V(\phi)$ in this class, they have obtained a general formula for the kink density which does not rely on details of the kink waveform or its small oscillations.

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