Classical statistical mechanics of one-dimensional polykink systems

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The phenomenological ideal-kink-gas theory recently developed by Currie, Krumhansl, Bishop, and Trullinger for the low-temperature statistical mechanics of one-dimensional, nonlinear, Klein-Gordon chains is extended and modified to treat systems capable of supporting more than one type of kink excitation. In particular, we consider a general class of local potentials that are doubly periodic, such as the double-sine-Gordon and doubly-periodic-quadratic cases, and support two different types of kinks having different creation energies. By taking into account topological restrictions on the sequencing of these two types of kinks (and their antikinks) along the chain, we find that the ideal-gas theory precisely reproduces results obtainable by the transfer-operator method. In addition, we present formulas for the low-temperature densities of kinks that depend only on quantities obtainable directly from the local potential and not on explicit knowledge of the waveforms of the kinks or their small oscillations.

I. INTRODUCTION

The statistical mechanics of one-component, one-dimensional systems governed by nonlinear on-site potentials that support kinklike solitary wave (soliton) solutions has recently been the subject of intensive study. Since the pioneering work of Krumhansl and Schrieffer,[1] which showed that the results of an exact transfer-operator treatment of the low-temperature statistical mechanics for the ϕ^4 potential could be explained remarkably well by a phenomenological model in which the kinks (solitons) behaved like an ideal gas, several workers have examined other soliton-bearing potentials[2-9] as well, refining both the transfer-operator[9,10] and phenomenological calculations.[2,3,5] As a result of these investigations, agreement between exact formalism and phenomenology (extending not only to temperature dependence but also to numerical prefactors) has been obtained for the double quadratic (DQ), ϕ^4, and sine-Gordon (SG) potentials[2] (see Fig. 1).

Encouraging as these results are, they are nevertheless somewhat limited in their applicability to real physical systems by the fact that all three of the potentials above, whether simple double wells (DQ, ϕ^4) or periodic (SG), possess only one type of potential barrier, and therefore can support only one type of kink solution (a kink being an excitation by which the relevant field evolves across a barrier from one minimum to an adjacent minimum). For wider generality, it is desirable to have a model that describes a "polykink" system, i.e., one for which more than one type of solitonic excitation is possible. One simple potential capable of supporting different solitonic solutions is a doubly periodic one (Fig. 2), which possesses two qualitatively different barriers and thus two distinct kink solutions. Such a doubly periodic potential (in the form of a double-sine-Gordon system) yields two types of solutions for magnetic solitons[11-13] in the B phase of superfluid ^{3}He. A doubly periodic potential is also the natural way for generalizing, to a lattice with diatomic bases, those lattice-dynamical models that assume simple singly periodic (usually sine-Gordon) potentials; among these are the model of

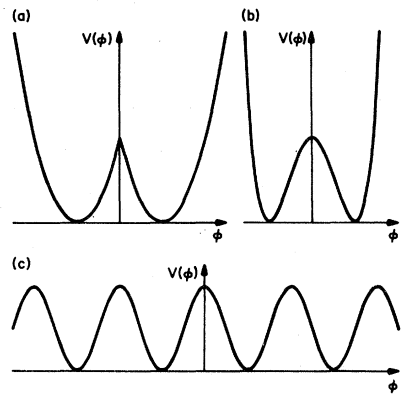

FIG. 1. Three examples of on-site potentials $V(\phi)$ that support one type of kinklike excitation. Note that all three possess at least two degenerate minima. (a) (double quadratic) and (b) (ϕ^4) are simple double wells. (c) (sine-Gordon) is periodic; note that all barriers are identical.

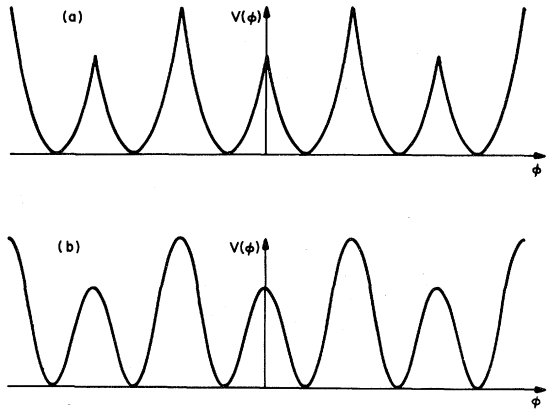

FIG. 2. Two examples of doubly periodic on-site potentials $V(\phi)$, which support two types of kinklike excitation. (a) doubly periodic quadratic (DPQ) and (b) double sine Gordon (DSG).

Frenkel and Kontorowa[14] for the motion of dislocations and that of Bishop[15] for the stationary sublattice in a quasi-one-dimensional superionic conductor.

The double-sine-Gordon (DSG) equation has been a useful model for disolitonic behavior, and analysis of soliton-soliton[11,16] and soliton-small-oscillation[12] scattering have been completed for the DSG potential. Despite this fairly extensive work on the dynamics of polykink systems, however, relatively little attention has been paid to their statistical mechanics. The purpose of this paper is to extend to potentials of double periodicity both the transfer-operator and phenomenological methods developed in Ref. 2 for calculation of the free energy of a one-dimensional (1D) chain with a singly periodic on-site potential, and to show, both in general and via two examples [DSG and doubly periodic quadratic (DPQ)—see Fig. 2], that the ideal-gas model gives precise agreement with the exact transfer-operator result at low temperatures. Before proceeding, we outline the symmetries of the class of doubly periodic potentials that we treat, and briefly outline how the methods of Ref. 2 can be extended to include polykink systems.

A useful lattice-potential analog of a doubly periodic potential is illustrated schematically by a chain of dimers in Fig. 3. We then have a simple generalization of a singly periodic lattice potential considered by Frenkel and Kontorowa[14] and by Bishop.[15] The potential $V(\phi)$ has the period of the lattice, and is symmetric about the midpoint of each dimer and about the midpoint between dimers, at

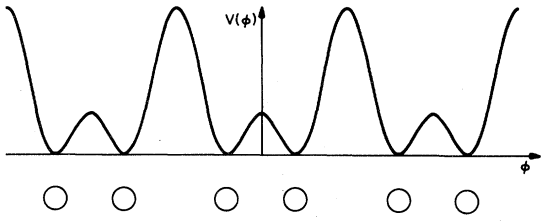

FIG. 3. Doubly periodic potential such as might be associated with a chain of dimerized atoms (underlying circles) in a quasi-one-dimensional material.

which points it has relative maxima. Thus, if the origin $\phi=0$ is taken at the middle of an intradimer barrier, and if the periodicity of the dimer chain is p, then $\phi=\frac{1}{2}p$ is the coordinate of the first maximum to the right of $\phi=0$ in the potential $V(\phi)$, and the features of $V(\phi)$ described above can be listed as follows:

$$V(\phi+p)=V(\phi)\,, \tag{1.1a}$$

$$V(-\phi)=V(\phi)\,, \tag{1.1b}$$

and

$$V(\tfrac{1}{2}p+(\phi-\tfrac{1}{2}p))=V(\tfrac{1}{2}p-(\phi-\tfrac{1}{2}p))\,, \tag{1.1c}$$

for periodicity, symmetry about an intradimer barrier, and symmetry about an interdimer barrier, respectively. The intradimer and interdimer barriers will hereafter be referred to as the type-I and type-II barriers, respectively; the first minimum to the right of the type-I barrier centered on the origin will be denoted by ϕ_1, so that the first type-II barrier to the right of $\phi=0$ will be centered at $\phi=\frac{1}{2}p$ and flanked by minima at ϕ_1 and $p-\phi_1\equiv\phi_2$.

In addition to the symmetries (1.1), the class of doubly periodic potentials $V(\phi)$ will be assumed to meet the following conditions:

Condition 1. (a) Local maxima of $V(\phi)$ are found only at

$$\phi=np,\ \ \phi=\tfrac{1}{2}p+np\,, \tag{1.2a}$$

while (b) local minima of $V(\phi)$ are found only at

$$\phi=\pm\phi_1+np,\ \ n=0,\pm1,\pm2,\ldots\,. \tag{1.2b}$$

Condition 2. The type-II (intradimer) barrier has greater "quantum-mechanical" strength than the type-I (intradimer) barrier; i.e., if $V(\phi)$ were a potential in a Schrödinger equation with very little effective mass (or $\hbar$ very small), the tunneling through barrier II would be weaker than that through barrier I. Mathematically,

$$\int_{\phi=0}^{\phi_1} d\phi \sqrt{V(\phi)} \equiv \mathscr{A}^{\mathrm{I}} < \mathscr{A}^{\mathrm{II}} ,$$
$$\mathscr{A}^{\mathrm{II}} \equiv \int_{\phi=p/2}^{\phi_2} d\phi \sqrt{V(\phi)} . \tag{1.3}$$

This relation will be important for the transfer-operator computation of statistical mechanical quantities.

Having defined the class of multikink potential to be dealt with, we briefly describe how the technique of Currie, Krumhansl, Bishop, and Trullinger[2] (hereafter referred to as CKBT) can be extended quite readily to the calculation of both the exact and phenomenological statistical mechanics of a disolitonic chain. The fundamental thermodynamic quantity of interest is the free energy. By a well-documented transfer-integral technique.[2,3,6,17] the free energy in the low-temperature limit is proportional to the lowest eigenvalue of an effective Schrödinger equation with very large effective mass; the potential in this equation is simply the particular nonlinear soliton-bearing potential $V(\phi)$ characterizing the system, and the solitonic contribution to the free energy can be readily associated with that component of the ground-state eigenvalue due to tunneling between wells of the potential. It is here that the second condition (1.3) above on $V(\phi)$ is relevant. A method for extending the transfer-integral formalism from the straightforward tunnel splitting of a double well to the more subtle tight-binding band structure of a singly periodic potential has recently been developed[2]; the extension to a doubly periodic calculation is then made quite easily, as it involves nothing more than a slight complication of the band structure.[9]

The basic features of the phenomenology developed by CKBT can be kept intact in an extension to systems with two types of solitons. The CKBT phenomenological model neglects kink-kink interactions, so that the only input required is the functional form and energy of each type of individual kink solution, along with the allowed forms for phonons in the presence of such a kink. The waveform and energy of a kink are determined only by the particular potential barrier spanned by the kink,[2] and by no features of the potential outside this barrier. Moreover, the symmetries of our class of doubly periodic potentials are such that the curvature of every well is the same, whence there is only one type of phonon; thus the treatment of the small-oscillation "dressing" that accompanies a kink can be carried over from CKBT. A new feature that enters the phenomenology for a double-kink system is a topological constraint on the manner in which the various types of kinks can be sequentially arranged in the system.

We consider a system consisting of a linear chain of harmonically coupled point masses, each of which moves in a doubly periodic potential (Fig. 3). We treat a general form of such a potential and illustrate the methods and results with the specific examples of double-sine-Gordon (DSG) and doubly periodic-quadratic (DPQ) cases. It is found in the low-temperature limit that the exact and phenomenological free energies for a general potential agree exactly.[9] We also consider relevant "kink-detecting" equal-time correlation functions; these too can be calculated both phenomenologically and exactly. Here it is also found that the two methods agree exactly at low temperatures. It thus appears that the ideal-gas picture for solitonic excitations, well established for single-kink systems, is also valid for those supporting two types of kink and, as probable consequence, for more than two types as well.

The details of the analysis establishing these results will be presented as follows. In Sec. II we consider a system with a general doubly periodic potential and discuss both the soliton solutions to the equation of motion and the small oscillations (phonons) in the presence of these kinks. We discuss the exact statistical mechanics of a doubly periodic chain in Sec. III via the transfer-operator technique; we exhibit the temperature dependence of the free energy in the low-temperature regime, and give the formal expressions for computing correlation functions. In Sec. IV we construct the phenomenology at low temperatures for a (topologically restricted) combined gas composed of two types of particles, which correspond to the two types of kinks as modified by a dressing of the accompanying phonon solutions discussed in Sec. II. The low-temperature free energy is computed and then compared to the exact expressions found in Sec. III. We also determine an appropriate kink-detecting function of ϕ, $F_i(\phi)$, for each type of soliton, and calculate the corresponding equal-time correlation functions $\langle F_i(\phi(0))F_i(\phi(x))\rangle$ by both exact and phenomenological methods. At each stage of this exposition, the general treatment is illustrated for two specific potentials. In Sec. V we conclude with a brief summary and suggestion of topics for future work.

II. EQUATION OF MOTION AND SOLITARY WAVE SOLUTIONS

In this section we consider the dynamics of a solitary wave-bearing system whose on-site potential

has the general doubly periodic form in Fig. 3; we also examine the two specific examples mentioned above. We present expressions for the two types of kink solutions, and discuss the phonon solutions in the presence of these kinks. The results of this section provide the basis for the phenomenological statistical mechanics discussed in Sec. IV.

The system under consideration consists of a one-dimensional chain of N harmonically coupled oscillators governed by the Hamiltonian[2] (in the notation of CKBT)

$$H=\sum_{i=1}^{N} lA\left[\frac{1}{2}\dot{\phi}_i^2+\frac{1}{2}\frac{c_0^2}{l^2}(\phi_{i+1}-\phi_i)^2+\omega_0^2 V(\phi_i)\right], \quad \phi_{N+1}\equiv\phi_1 \tag{2.1}$$

where ϕ_i is the dimensionless "displacement" coordinate of the ith oscillator, l the equilibrium spacing between nearest neighbors, and $V(\phi)$ a dimensionless "on-site" potential of the doubly periodic form described in Sec. I. In addition to the symmetries (1.1) and features (1.2), $V(\phi)$ will also be assumed for convenience to possess the following properties:

$$V(np\pm\phi_1)=0 \tag{2.2a}$$

and

$$V''(\pm\phi_1+np)=1 \quad (n=0,\pm1,\pm2,\ldots). \tag{2.2b}$$

Equation (2.2a) ensures that $V(\phi)$ is everywhere non-negative, with the arbitrary zero of potential energy chosen so that $V(\phi)$ is zero at all its (degenerate) minima; (2.2b) normalizes to unity the curvature of $V(\phi)$ at all its minima.

Two specific examples of such potentials are (see Fig. 2) the following: (1) DPQ,

$$V(\phi)=\tfrac{1}{2}(|\phi|-1)^2, \quad |\phi|<\phi_0$$
$$V(\phi+2\phi_0)=V(\phi), \quad \phi_0\geq 2 \tag{2.3a}$$

($\phi_0=2$ gives a degenerate, or singly periodic, case with period ϕ_0), and (2) DSG,

$$V(\phi)=\frac{2}{1-\alpha^2}\left[\cos\left[\frac{\phi}{2}\right]-\alpha\right]^2, \quad 0\leq\alpha<1 \tag{2.3b}$$

[$\alpha=0$ gives a degenerate (sine-Gordon) case with period 2π; otherwise the period is 4π.]

We restrict the range of the parameters in (2.1) to the "displacive" limit, in which the length $d\equiv c_0/\omega_0$ satisfies the inequality $d\gg l$, thereby making the coupling between sites strong enough to ensure that variations of ϕ from site to site are quite small, at least at low temperatures. It is in this displacive regime that nonlinear kinks become well-defined[18] elementary excitations with long lifetimes and as such behave[19] very much like particles. In this limit the Hamiltonian (2.1) becomes

$$H=A\int_{x=0}^{L\equiv Nl} dx\{\tfrac{1}{2}[\dot{\phi}(x,t)]^2+\tfrac{1}{2}c_0^2[\phi_x(x,t)]^2+\omega_0^2 V(\phi)\}. \tag{2.4}$$

Both forms (2.1) and (2.4) of the Hamiltonian will be utilized in our analysis. The discrete form (2.1) is used in obtaining exact statistical-mechanical results via the transfer-operator formalism, whereupon the process of taking the continuum limit afterwards becomes explicit. The continuum form (2.4) is used to study the nature of the solitary wave (kink) and linear (phonon) excitations of the system. It is these excitations that are introduced into the statistical mechanics through the "kink-gas" phenomenology in Sec. IV.

The Euler-Lagrange equation of motion following from (2.4) is

$$\phi_{tt}-c_0^2\phi_{xx}+\omega_0^2\frac{dV}{d\phi}=0. \tag{2.5}$$

We begin by examining the solitary wave solutions, first finding static kink waveforms $\phi_i^0(x)$. (The subscript $i=$I, II distinguishes the two types of kinks in the system.) The "Lorentz" covariance of (2.4) implies a whole family of traveling kinks:

$$\phi_i^{(v)}(x,t)\equiv\phi_i^{(0)}(\gamma(x-vt)),$$

where $\gamma\equiv[1-(v/c_0)^2]^{-1/2}$. We define the nth type-I (smaller) barrier in $V(\phi)$ as that barrier spanning the range of ϕ defined by $-\phi_1+np<\phi<\phi_1+np$, $n=0,\pm1,\pm2,\ldots$; similarly, the nth type-II (larger) barrier in $V(\phi)$ spans that region for which $\phi_1+np<\phi<(n+1)p-\phi_1$. [$\phi_1$ is defined following Eqs. (1.1).] A kink excitation $\phi_{i\pm}^{(0)}(\gamma(x-vt))$ evolves the system between two minima flanking a barrier of type i ($i=$I, II), with the $+(-)$ sign denoting that the excitation is an increasing (decreasing) function of $s\equiv x-vt$, and hence a kink (antikink).

The general formalism for obtaining solitonic solutions to an equation of the type (2.5) is presented in Ref. 2; we give here only those results for the two specific example potentials which we consider. By convention, we always take $\phi_{\mathrm{I}\pm}^{(0)}(x=0)=np$, $\phi_{\mathrm{II}\pm}^{(0)}(x=0)=(n+\frac{1}{2})p$ for some integer n. For DPQ,[2,5]

$$\phi_{\mathrm{I}\pm}^{(v)}(x,t)=2n\phi_0\pm\mathrm{sgn}(x-vt)\left[1-\exp\left[-\frac{\gamma|x-vt|}{d}\right]\right]. \tag{2.6}$$

$$\phi_{\mathrm{II}\pm}^{(v)}(x,t)=(2n+1)\phi_0\pm\mathrm{sgn}(x-vt)(\phi_0-1)\left[1-\exp\left[-\frac{\gamma|x-vt|}{d}\right]\right]. \tag{2.7}$$

For DSG,[11,12]

$$\phi_{\mathrm{I}\pm}^{(v)}(x,t)=4\pi n\pm 4\tan^{-1}\left[\left[\frac{1-\alpha}{1+\alpha}\right]^{1/2}\tanh\left[\frac{\gamma(x-vt)}{2d}\right]\right], \tag{2.8}$$

$$\phi_{\mathrm{II}\pm}^{(v)}(x,t)=(2n+1)(2\pi)\pm 4\tan^{-1}\left[\left[\frac{1+\alpha}{1-\alpha}\right]^{1/2}\tanh\left[\frac{\gamma(x-vt)}{2d}\right]\right]. \tag{2.9}$$

Sketches of the waveforms (2.6)–(2.9) are given in Fig. 4. All these waveforms are such that $\phi_{i\pm}^{(v)}(s)-\phi_{i\pm}^{(v)}(0)$ possesses odd parity[$s\equiv\gamma(x-vt)$]:

$$\phi_{i\pm}^{(v)}(-s)-\phi_{i\pm}^{(v)}(0)=-[\phi_{i\pm}^{(v)}(s)-\phi_{i\pm}^{(v)}(0)]. \tag{2.10}$$

Equation (2.10) is a consequence of the symmetry properties (1.1), the equation of motion (2.5), and the convention mentioned just before Eq. (2.6).

Just as the functional form of a general solitonic excitation reflects the Lorentz covariance of (2.5), so too does the expression for the kink energy $E_i^{(v)}$, which is given by[2,3,5]

$$E_i^{(v)}=\gamma E_i^{(0)}=(E_i^{(0)2}+p_i^2c_0^2)^{1/2}. \tag{2.11}$$

Here the kink rest energy $E_i^{(0)}$ and momentum p_i are given by $E_i^{(0)}\equiv M_ic_0^2$ and $p_i\equiv\gamma M_iv$ with[2]

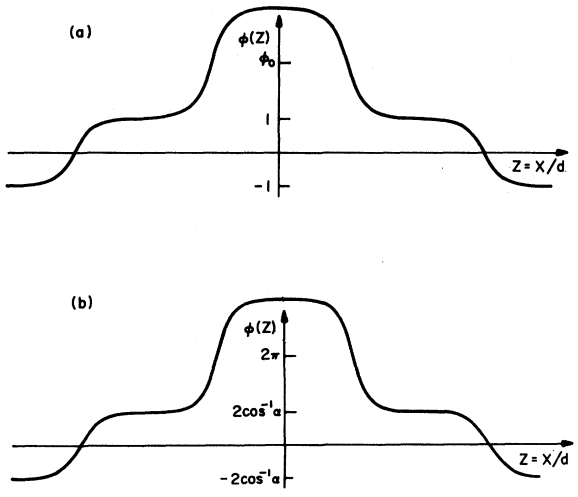

FIG. 4. Sketches of the four possible kinklike excitations in a doubly periodic system for the (a) doubly-periodic-quadratic (DPQ) and (b) double-sine-Gordon (DSG) potentials. In both cases the sequence of excitations, from left to right, is as follows: type-I kink, type-II kink, type-II antikink, type-I antikink.

$$M_i\equiv\frac{E_i^{(0)}}{c_0^2}=\frac{2A}{d^2}\int_{-\infty}^{+\infty}dx\,V(\phi_{i\pm}^{(0)}(x))$$
$$=\frac{2\sqrt{2A}}{d}\mathscr{A}^i, \tag{2.12}$$

where the $\mathscr{A}^i$ are defined in (1.3). For our examples, the various kink rest masses are (i) for DPQ (Refs. 2, 3, and 5),

$$M_{\mathrm{I}}=\frac{A}{d},\quad M_{\mathrm{II}}=\frac{A}{d}(\phi_0-1)^2, \tag{2.13a}$$

and (ii) for DSG (Refs. 11 and 12),

$$M_{\mathrm{I}}=\frac{8}{(1-\alpha^2)^{1/2}}\frac{A}{d}\left[(1-\alpha^2)+\alpha\arcsin\alpha-\frac{\pi}{2}\alpha\right], \tag{2.13b}$$

$$M_{\mathrm{II}}=\frac{8}{(1-\alpha^2)^{1/2}}\frac{A}{d}\left[(1-\alpha^2)^{1/2}+\alpha\arcsin\alpha+\frac{\pi}{2}\alpha\right].$$

We now examine the second set of solutions to (2.5) that concerns us; these are the small-amplitude oscillations of the system, which are very different in both form and physical import from the large-amplitude kink solutions. Moreover, because an understanding of the kink-phonon interaction is essential to a correct phenomenology,[2] we must find the form of the small oscillations *in the presence of a kink;* more precisely, it is the asymptotic form, as $|x|\to\infty$, of these perturbed phonons that enters the phenomenological calculation.[2] We therefore consider the effects of a single kink on the small-amplitude solutions, working for convenience in the kink rest frame. By assuming the small oscillation to be of the form

$$\chi(x,t)\equiv f(x)\cos(\omega t), \tag{2.14}$$

the standard linearization of (2.5) gives the following effective Schrödinger equation for the spatial factor of χ:

$$-c_0^2 f''(x)+\omega_0^2 U_i(x) f(x)=\omega^2 f(x) , \tag{2.15}$$

where

$$U_i(x)\equiv V''(\phi_{i\pm}^{(0)}(x)) \tag{2.16}$$

is the dimensionless effective potential. [We have explicitly indicated by the $\pm$ subscript on $\phi_i^{(0)}$ that $U_i(x)$ has the same form whether it results from a kink or an antikink.]

The "scattering potentials" $U_i(x)$ have certain basic features in common,[2] the most important of which are

$$U_i(x=0)<0 \tag{2.17}$$

and

$$U_i(\,|x|\to\infty)\to 1 . \tag{2.18}$$

Furthermore, the odd parity of the quantity $\phi_{i\pm}^{(0)}(x)-\phi_{i\pm}^{(0)}(0)$, along with the symmetry properties (1.1) for the potential $V(\phi)$, implies that

$$U_i(-x)=U_i(x) . \tag{2.19}$$

Each type of kink thus presents the phonons with a potential well in one dimension. The explicit forms of these scattering potentials for both types of DPQ and DSG kinks are given in Table I.

A few features of these formulas deserve some comment. The delta functions in $U_i(x)$ for the DPQ case result from the the cusps in $V(\phi)$ (Ref. 5); also, although the delta function in $V''(\phi)$ has a larger amplitude by a factor of ϕ_0-1 for the type-II barrier than for the type-I barrier, Eqs. (2.6) and (2.7) show that $\phi_{\rm II}^{(0)'}(x)$ is larger than $\phi_{\rm I}^{(0)'}(x)$ by the same factor. Thus, loosely speaking, the increase in the depth of $U_{\rm II}(x)$ over that of $U_{\rm I}(x)$ is offset by a corresponding reduction of the width in x of $U_{\rm II}(x)$; this leads to the precise equality for the scattering potentials of the two DPQ kinks that the table displays.

The expression for either of the DSG scattering potentials can be obtained from the other by sending α to $-\alpha$; for all values of α, the two scattering potentials exhibit a basic qualitative difference, in that $U_{\rm I}(x)$ increases monotonically as x increases from 0 to $+\infty$, while $U_{\rm II}(x)$ possesses "shoulders"[12] peaked at points $x=\pm x_0(\alpha)$ such that $U_{\rm II}(x=\pm x_0(\alpha))>1$. Figure 5 shows this behavior for three values of α.

Regardless of the precise form of $U_i(x)$, some remarks of a general nature can be made concerning the eigenfunctions $f(x)$ of Eq. (2.15). We can classify the functions $f(x)$ into two main categories: bound (localized) modes with $\omega^2<\omega_0^2$, and scattering (extended) modes with $\omega^2>\omega_0^2$. The translational invariance of the Hamiltonian (2.4) guarantees[20] that $\phi_{i\pm}^{(0)'}(x)$, the Goldstone mode, satisfies (2.15) with $\omega^2=\omega_{i,1}^2=0$; this zero-frequency solution is the ground state for the potential $U_i(x)$. In addition to this translation mode, there may be additional bound states with frequencies $\omega_{i,n}$ such that $0<\omega_{i,n}^2<\omega_0^2$, $n\geq 2$. These are internal oscillations of the kink that are treated as localized phonons in the phenomenology.

Expressions for the translational modes $f_{b,1}^{(i)}(x)$ associated with each of the kinks in the systems under consideration, normalized according to

$$\int_{-\infty}^{\infty} dx[f_{b,1}^{(i)}(x)]^2=1 ,$$

are given in Table II. This is the only localized mode for the DPQ kinks, since an attractive delta-function potential has exactly one bound state. We were unable to determine analytically the presence or nature of higher bound states for the scattering potentials associated with the DSG kinks; instead, we searched for such modes by solving Eq. (2.15) numerically for all values $\alpha=0.05\times n$, $n=1,2,3,\ldots,19$. The results indicate that there are no higher bound states for the $U_{\rm II}(x)$ DSG potential, and exactly one higher bound state for $U_{\rm I}(x)$. In Fig. 6 we plot this frequency, $\omega_{\rm I,2}$, as a function of α. In Fig. 5 we plot the scattering potentials and their bound-state waveforms for DSG kinks for three values of α, again with the normalization

$$\int_{-\infty}^{\infty} dx[f_{b,n}^{(i)}(x)]^2=1 .$$

TABLE I. Forms of the scattering potentials $U_i(x)\equiv V''(\phi_{i\pm}^{(0)}(x))$ (i refers to the type of kink, and can be either I or II) for each of the two example systems considered. Note that $U_{\rm I}(x)=U_{\rm II}(x)$ for the doubly-periodic-quadratic (DPQ) case, and that $U_{\rm I}(x)$ and $U_{\rm II}(x)$ are related by the transformation $\alpha\to-\alpha$ in the double-sine-Gordon (DSG) case.

	Type I	Type II
DPQ	$1-2\delta(x/d)$	$1-2\delta(x/d)$
DSG	$1-\dfrac{3\alpha}{\cosh(x/d)+\alpha}-\dfrac{2(1-\alpha^2)}{[\cosh(x/d)+\alpha]^2}$	$1+\dfrac{3\alpha}{\cosh(x/d)-\alpha}-\dfrac{2(1-\alpha^2)}{[\cosh(x/d)-\alpha]^2}$

TABLE II. Forms of the ground-state (translation mode) eigenstates $f_{b,1}^{(i)}(x)$ for the potentials $U_i(x)$ in Eq. (2.15). The normalization condition $\int_{-\infty}^{+\infty} dx[f_{b,1}^{(i)}(x)]^2=1$ is used, and the superscript i refers to the type (I or II) of kink. As for the scattering potentials $U_i(x)$ in Table I, $f_{b,1}^{(I)}(x)=f_{b,1}^{(III)}(x)$ for the doubly-periodic-quadratic system, while $f_{b,1}^{(I)}(x)$ and $f_{b,2}^{(II)}(x)$ are related by the transformation $\alpha\rightarrow-\alpha$ in the double-sine-Gordon case.

	Type I	Type II
DPQ	$f_{b,1}^{(I)}(x)=\frac{1}{\sqrt{d}}\exp\left[-\frac{\lvert x\rvert}{d}\right]$	$f_{b,1}^{(III)}(x)=\frac{1}{\sqrt{d}}\exp\left[-\frac{\lvert x\rvert}{d}\right]$
DSG	$f_{b,1}^{(I)}(x)=\left[\frac{1-\alpha^2}{2d}\right]^{1/2}\left[1-\frac{\alpha\cos^{-1}\alpha}{(1-\alpha^2)^{1/2}}\right]^{-1/2}\frac{1}{\cosh(x/d)+\alpha}$	$f_{b,1}^{(III)}(x)=\left[\frac{1-\alpha^2}{2d}\right]^{1/2}\left[1+\frac{\alpha\cos^{-1}\alpha}{(1-\alpha^2)^{1/2}}\right]^{-1/2}\frac{1}{\cosh(x/d)-\alpha}$

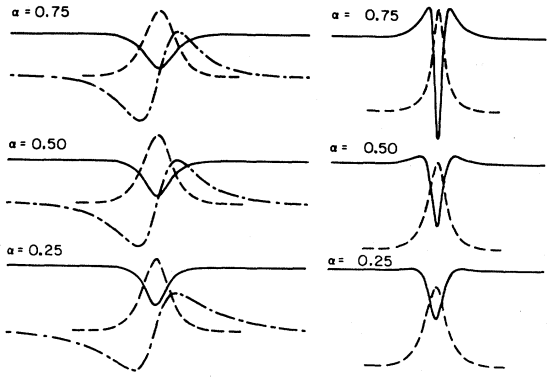

FIG. 5. Plots of the perturbing potentials (solid lines) experienced by phonons in the presence of double-sine-Gordon kinks for various values of the parameter α. The corresponding "translation mode" ground states (dashed lines) and excited bound states (for type I; dashed-dotted lines) are also shown. The plots on the left are associated with type-I kinks and those on the right with type-II kinks.

Turning now to the scattering (extended) solutions $f_k^{(i)}(x)$ of Eq. (2.15), we note that (2.18) implies the following asymptotic behavior:

$$f_k^{(i)}(x)\underset{x\rightarrow\pm\infty}{\rightarrow}a_{1\pm}^{(i)}\cos(kx)+a_{2\pm}^{(i)}\sin(kx)\ . \quad (2.20)$$

Only two of the four coefficients $a_{j\pm}^{(i)}$ are independent (for a given kink type i), the relationships among them being expressible by basic scattering formalism. The wave vector k and the eigenvalue $\omega^2=\omega_k^2$ are related by the continuum dispersion relation for unperturbed phonons,

$$\omega_k^2=\omega_0^2+c_0^2k^2\ . \quad (2.21)$$

The symmetry (2.19) indicates that the appropriate set of extended solutions $f(x)$ are those with definite parity,[5] the even and odd members of which exhibit the following asymptotic behavior, respectively:

$$f_k^+(x)\underset{x\rightarrow\pm\infty}{\rightarrow}\cos[kx\pm\tfrac{1}{2}\Delta^+(k)] \quad (2.22a)$$

and

$$f_k^-(x)\underset{x\rightarrow\pm\infty}{\rightarrow}\sin[kx\pm\tfrac{1}{2}\Delta^-(k)]\ . \quad (2.22b)$$

$\Delta^+(k)$ and $\Delta^-(k)$ are the k-dependent phase shifts associated, respectively, with the even and odd "standing-wave" states of wave vector k. All information concerning the scattering states needed for the phenomenology is contained in $\Delta^{\pm}(k)$. Before presenting the phenomenological formalism, howev-

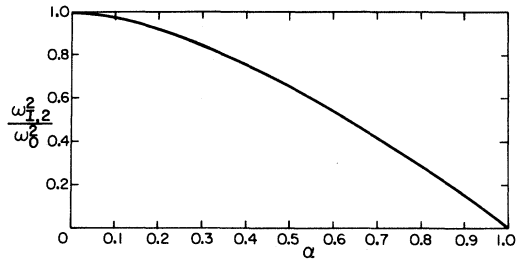

FIG. 6. Square of the normalized frequency $(\omega_{I,2}/\omega_0)^2$ of the internal oscillation of the type-I double-sine-Gordon kink is plotted as a function of α.

er, we next consider the exact transfer-operator method for obtaining thermodynamic functions.

III. EXACT STATISTICAL MECHANICS

The classical partition function Z for the system described by the Hamiltonian (2.1) factors into kinetic and configurational parts,[2,3,5]

$$Z=Z_{\dot{\phi}}Z_{\phi} . \tag{3.1}$$

The kinetic factor is given by[2]

$$Z_{\dot{\phi}}=(2\pi Al/\beta h^2)^{N/2} , \tag{3.2}$$

where h is Planck's constant. Z_{ϕ} can be evaluated by a well-documented transfer-integral technique,[1-3,6,18] and is given in the thermodynamic limit, for both unbounded and periodic potentials, by

$$Z_{\phi}=\exp(-\beta A\omega_0^2 L\epsilon_0) , \tag{3.3}$$

where ϵ_0 is the lowest eigenvalue of a transfer-integral operator involving the strain and on-site potential energy terms in the Hamiltonian. In the displacive regime ($l \ll d$) under study, the transfer-integral eigenvalues ϵ are those of the effective Schrödinger equation[2]

$$-\frac{1}{2m^*}\frac{d^2\psi(\phi)}{d\phi^2}+V(\phi)\psi(\phi)=(\epsilon-V_0)\psi(\phi) , \tag{3.4}$$

$$m^*\equiv(A\omega_0 c_0\beta)^2=\left[\frac{\beta E_i^{(0)}}{2\sqrt{2}\mathscr{A}^i}\right]^2 , \quad i=\mathrm{I,II} . \tag{3.5}$$

V_0 is a temperature-dependent zero of "energy" that is independent of the form of $V(\phi)$. We consider the limit in which the thermal energy is much less than the kink rest energy. Hence, the dimensionless effective mass m^* is very large, so that the ground-state eigenvalue ϵ_0 is given by[1-3,9,21,22]

$$\epsilon_0=V_0+\tfrac{1}{2}m^{*-1/2}+a(m^{*-1})-t_0 . \tag{3.6}$$

$\frac{1}{2}m^{*-1/2}$ is the lowest ($n=0$) harmonic level of a single well of $V(\phi)$ (recall that all wells have the same curvature), $a(m^{*-1})$ represents a shift smaller in magnitude than a constant times m^{*-g}, $g\geq 1$, due to the anharmonicity of a single well,[9,21] and $t_0>0$ is a splitting, exponentially small in $m^{*1/2}$, due to the very weak tunneling between wells for large m^*. The free energy per unit length is thus

$$\begin{aligned} f&=-\frac{k_BT}{L}\ln Z \\ &=-\frac{k_BT}{L}\ln Z_{\dot{\phi}}+A\omega_0^2\epsilon_0 \\ &=-\frac{k_BT}{L}\ln Z_{\dot{\phi}}+A\omega_0^2V_0+\frac{1}{2}\frac{k_BT}{d} \\ &\quad +A\omega_0^2a(m^{*-1})-A\omega_0^2t_0 . \end{aligned} \tag{3.7}$$

The sum of the first three terms on the right-hand side of (3.7), for any $V(\phi)$,[2,9] is precisely equal to the free energy density of a set of one-dimensional classical harmonic phonons when calculated to the order $O(l/d)$ of the displacive approximation by using the discrete-lattice dispersion relation.[2] The anharmonic $a(m^{*-1})$ term is as yet unaccounted for by any quantitative phenomenology, but the tunneling term $-A\omega_0^2t_0$, just as for those potentials supporting only one type of kink,[2,3,9] can be clearly associated with the kinks; it is therefore on this term that we shall focus our attention. Specifically, the leading term at very low T in the tunneling component for the free-energy density of a doubly periodic potential is given by[9]

$$\begin{aligned} f_t&=-A\omega_0^2t_0 \\ &=-A\omega_0^2(t_0^{\mathrm{I}}+t_0^{\mathrm{II}}) , \end{aligned} \tag{3.8}$$

where

$$t_0^{\mathrm{I}}=\frac{1}{\sqrt{\pi}}\left[\frac{k_BT}{A\omega_0c_0}\right]^{1/2}\phi_1 e^{\eta_{\mathrm{I}}}\exp(-\beta E_{\mathrm{I}}^{(0)}) \tag{3.9a}$$

and

$$t_0^{\mathrm{II}}=\frac{1}{\sqrt{\pi}}\left[\frac{k_BT}{A\omega_0c_0}\right]^{1/2}\left[\frac{p}{2}-\phi_1\right]e^{\eta_{\mathrm{II}}} \times\exp(-\beta E_{\mathrm{II}}^{(0)}) . \tag{3.9b}$$

The η_i are numerical constants, whose dependence on the potential is as follows:

$$\eta_{\rm I} \equiv \int_0^{\phi_1} d\phi\, g_{\rm I}(\phi)\,, \tag{3.10a}$$

$$g_{\rm I}(\phi) \equiv [2V(\phi)]^{-1/2} - (\phi_1 - \phi)^{-1}$$

$$\eta_{\rm II} \equiv \int_{p/2}^{p-\phi_1} d\phi\, g_{\rm II}(\phi)\,, \tag{3.10b}$$

$$g_{\rm II}(\phi) \equiv [2V(\phi)]^{-1/2} - (p - \phi_1 - \phi)^{-1}\,.$$

All temperature dependence of (3.8) can be obtained by keeping lowest order terms in a WKB analysis of (3.4),[9] the emergence of the Boltzmann factors $\exp(-\beta E_i^{(0)})$ from such a treatment being strongly foreshadowed by the proportionality of the soliton rest energies to the expressions $\mathscr{A}^i$ defined in Eq. (1.3). The numerical prefactor $1/\sqrt{\pi}$ in $t_0^{\rm I}$ and $t_0^{\rm II}$ is the result of a technique whch is a modification and generalization[9,10,21,22] of Goldstein's method[23] for determination of the bandwidths for the characteristic numbers (eigenvalues) of the Mathieu equation for that range of parameters in which the Mathieu equation becomes (3.4) with $V(\phi)=1+\cos\phi$ and $m^* \gg 1$. The same numerical correction factor for WKB has been found in similar double-well and singly periodic problems by other workers.[21,22,24–34] Especially important in this connection are two papers[21,22] by Harrell, which provide rigorous mathematical proof for these results.

Below we examine the features of the band structure, in the limit of very large m^*, for the effective Schrödinger equation (3.4) when $V(\phi)$ is a doubly periodic potential. An understanding of these features is very helpful in motivating the plausibility and generality of the result (3.8); moreover, detailed knowledge of this structure is essential for the computation of equal-time site-site correlation functions.[2,9] Below, then, we examine the "tight-binding band structure" of a general "dimer-based" potential, by using the analogy with a "one-electron problem."

The problem is to approximate with sufficient accuracy the solutions to the Schrödinger equation for an "electron" moving in the 1D potential due to the "atoms" of the molecular chain in Fig. 7. Although the eigenstates of such a potential are Bloch functions, for the tight-binding limit that we consider the "electron density" will be so highly localized in the troughs of the potential that the problem is most conveniently analyzed in terms of the molecular orbitals of the free diatomic molecules; this is essentially the same viewpoint as would be applied to a singly periodic chain, except that here we deal with molecular instead of atomic orbitals. For a dimer, a molecular orbital is of course a linear combination of the atomic orbitals from the individual atoms comprising the dimer, so that the problem is only slightly more complicated than that for the singly periodic case. We focus our attention on the two lowest bands, which are all that are needed to compute the relevant kink-detecting correlation functions. The main points in the ensuing discussion are illustrated by Figs. 7 and 8.

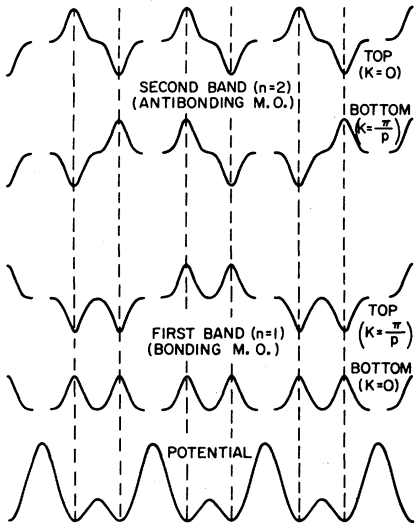

FIG. 7. Schematic sketch of tight-binding (high effective mass) wave functions at the zone center ($k=0$) and zone edge ($k=\pi/p$) for the two lowest bands of a doubly periodic potential with period p. If one considers the potential to be associated with a chain of dimers like that in Fig. 3, the states of the lower band are formed from bonding molecular orbitals, while those of the upper band are formed from antibonding molecular orbitals.

For the regime of very large effective mass m^* in which we work, the overlap of the wave function between molecules will be so small that near each dimer the moduli of the eigenfunctions of the two lowest bands will be proportional to the moduli of the two lowest-lying molecular orbitals; each of these two molecular orbitals is in turn a different linear combination of the ground-state atomic orbitals. For this "dimer-based" 1D system, these lowest atomic orbitals are simply the ground-state harmonic-oscillator functions for a single well of $V(\phi)$; this accounts for the "harmonic" term $\frac{1}{2}m^{*1/2}$ in Eq. (3.6). The lower band is based on the molecular orbital which is a symmetric (bonding) combination of the atomic orbitals (Fig. 7, bottom); the upper band arises from the antisymmetric (antibonding) state (Fig. 7, top). The gap between these bands is therefore due to tunneling through

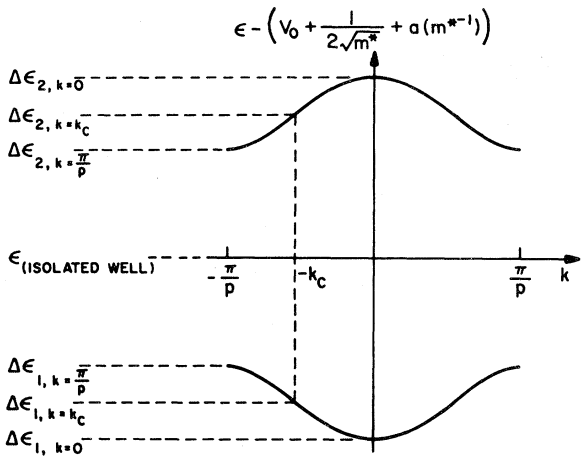

FIG. 8. Structure of the two lowest bands of eigenvalues ϵ in Eq. (3.4) for a doubly periodic potential $V(\phi)$ of period p and for very large m^*. The deviation $\Delta\epsilon_{n,k}$ (n is the band index) from the isolated-well eigenvalue is plotted as a function of wave vector k in the reduced-zone scheme. Note the symmetries $\Delta\epsilon_{1,k}=-\Delta\epsilon_{2,k}, \Delta\epsilon_{n,-k}=\Delta\epsilon_{n,k}$. The wave vector k_c locates the band center. The band gap is due to tunneling effects associated with the smaller (type-I) barrier, while the bandwidths are due to the weaker tunneling effects associated with the larger (type-II) barrier.

the smaller (type-I) barrier between atoms of the same dimer; this band gap gives rise to the t_0^{I} term in (3.8). The t_0^{II} term arises from the width of an individual band. This can be seen most readily when the states are written in Bloch form[2] in the reduced-zone scheme,

$$\psi_{n,k}(\phi)=u_{n,k}(\phi)e^{ik\phi}\ ,$$
$$u_{n,k}(\phi+p)=u_{n,k}(\phi)\ . \tag{3.11}$$

Here $-\pi/p<k\leq\pi/p$, and $n\geq 1$ is an integral band index. $|u_{n,k}(\phi)|$ is practically independent of k in this large-m^* regime, so that the probability density $|u_{n,k}(\phi)|^2$ is essentially that of the molecular orbital from which the nth band is built. The lowest state within the bonding ($n=1$) band is symmetric with respect to the larger interdimer type-II barrier and thus has $k=0$; the highest state within this bonding band is antisymmetric with respect to the type-II barrier and therefore has period $2p$, whence k ($=\pi/p$) is at the zone edge. The bandwidth is thus determined by the tunneling through the type-II barrier; as mentioned earlier, this type-II tunneling is weaker than the type-I tunneling, and we obtain self-consistently that the bandwidth is less than the band splitting. The upper antibonding ($n=2$) band similarly will have a width proportional to the type-II tunneling, although the k dependence in this band is inverted from that of the lower band. This is because the lowest state is symmetric with respect to the type-II barrier, but the antibonding orbital's antisymmetry about the type-I barrier gives this state a period $2p$, so that $k=\pi/p$; the highest state in the $n=2$ band is antisymmetric with respect to both barriers, and therefore has the periodicity of the potential, so that $k=0$. Figure 8 displays the qualitative features of the structure of these two lowest bands.

When this structure is analyzed quantitatively through the generalized method of Ref. 23, one obtains the full k-dependent forms[9] of (3.8) for the two lowest bands. Defining

$$\epsilon_{n,k}=\tfrac{1}{2}m^{*-1/2}+a(m^{*-1})+\Delta\epsilon_{n,k}\ , \tag{3.12}$$

where $n=1,2$ are the band indices used above, we find that

$$\begin{aligned}A\omega_0^2\Delta\epsilon_{1,k}&=-A\omega_0^2\Delta\epsilon_{2,k}\\&=-\frac{1}{\sqrt{\pi}}\left[\frac{A\omega_0 c_0}{d}\right]\left[\frac{k_BT}{A\omega_0 c_0}\right]^{1/2}\\&\times\left\{\left[\phi_1 e^{\eta_{\mathrm{I}}}\exp(-\beta E_{\mathrm{I}}^{(0)})-\left[\frac{p}{2}-\phi_1\right]e^{\eta_{\mathrm{II}}}\exp(-\beta E_{\mathrm{II}}^{(0)})\right]^2\right.\\&\left.+4\phi_1\left[\frac{p}{2}-\phi_1\right]\exp(\eta_{\mathrm{I}}+\eta_{\mathrm{II}})\exp[-\beta(E_{\mathrm{I}}^{(0)}+E_{\mathrm{II}}^{(0)})]\cos^2(\tfrac{1}{2}pk)\right\}^{1/2}\ ,\quad -\frac{\pi}{p}<k\leq\frac{\pi}{p}\ .\end{aligned} \tag{3.13}$$

Each bandwidth is given by ($k_{\mathrm{BZ}}\equiv\pi/p$)

$$|\Delta\epsilon_{n,k_{\mathrm{BZ}}}-\Delta\epsilon_{n,k=0}|=2t_0^{\mathrm{II}}\ , \tag{3.14}$$

where BZ denotes the Brillouin-zone boundary, while the splitting between band centers is given by

$$\Delta\epsilon_{2,k_c}-\Delta\epsilon_{1,k_c}=2t_0^{\mathrm{I}}\ , \tag{3.15}$$

where k_c is defined as the wave vector for which

$$\Delta\epsilon_{n,k_c}=\tfrac{1}{2}(\Delta\epsilon_{n,k_{BZ}}+\Delta\epsilon_{n,k=0}) , \tag{3.16}$$

so that

$$\cos^2(\tfrac{1}{2}pk_c)=\frac{1}{2}-\frac{1}{4}\left[\frac{p}{2}-\phi_1\right]^{-1}\phi_1\exp(\eta_{\rm I}+\eta_{\rm II}) \times\exp[-\beta(E_{\rm II}^{(0)}-E_{\rm I}^{(0)})] . \tag{3.17}$$

[$k_c\simeq\pm\frac{1}{2}(\pi/p)$ if the thermal energy is much less than the difference in kink rest energies.] The reader is referred to Fig. 8 for an illustration of these features.

For the two examples under consideration, we have explicitly, for DPQ,

$$A\omega_0^2\Delta\epsilon_{1,k}=-\frac{1}{\sqrt{\pi}}\frac{A\omega_0c_0}{d}\left[\frac{k_BT}{A\omega_0c_0}\right]^{1/2}\{[\exp(-\beta E_{\rm I}^{(0)})-(\phi_0-1)\exp(-\beta E_{\rm II}^{(0)})]^2 +4(\phi_0-1)\cos^2(\tfrac{1}{2}pk)\exp[-\beta(E_{\rm I}^{(0)}+E_{\rm II}^{(0)})]\}^{1/2} , \tag{3.18a}$$

and for DSG,

$$A\omega_0^2\Delta\epsilon_{1,k}=-\frac{(1-\alpha^2)^{1/2}}{\sqrt{\pi}}\frac{A\omega_0c_0}{d}\left[\frac{k_BT}{A\omega_0c_0}\right]^{1/2}\{[\exp(-\beta E_{\rm I}^{(0)})-\exp(-\beta E_{\rm II}^{(0)})]^2 +4\cos^2(\tfrac{1}{2}pk)\exp[-\beta(E_{\rm I}^{(0)}+E_{\rm II}^{(0)})]\}^{1/2} . \tag{3.18b}$$

Specializing Eqs. (3.18) to the value $k=0$, which gives the ground state of the potential, we find the tunneling free energy densities for the two systems:

$$(f_t)_{\rm DPQ}=-\frac{1}{\sqrt{\pi}}\left[\frac{A\omega_0c_0}{d}\right]\left[\frac{k_BT}{A\omega_0c_0}\right]^{1/2}[\exp(-\beta E_{\rm I}^{(0)})+(\phi_0-1)\exp(-\beta E_{\rm II}^{(0)})] \tag{3.19a}$$

and

$$(f_t)_{\rm DSG}=-\frac{(1-\alpha^2)^{1/2}}{\sqrt{\pi}}\left[\frac{A\omega_0c_0}{d}\right]\left[\frac{k_BT}{A\omega_0c_0}\right]^{1/2}[\exp(-\beta E_{\rm I}^{(0)})+\exp(-\beta E_{\rm II}^{(0)})] . \tag{3.19b}$$

These will be compared to the phenomenological results in Sec. IV.

We now give the general expression for the equal-time thermal average of the correlation in the values of some function $F(\phi)$ between two different sites on the chain of mass points. Specifically, in the thermodynamic limit $L\to\infty$ the correlation in $F(\phi)$ between two sites indexed by j and m is given by

$$\langle F(\phi_j)F(\phi_m)\rangle=\frac{p}{2\pi}\sum_{n=1}^{\infty}\int_{-\pi/p}^{\pi/p}dk\,\langle n'=1,k'=0\,|\,F(\phi)\,|\,n,k\rangle\langle n,k\,|\,F(\phi)\,|\,n''=1,k''=0\rangle_N \times\exp[-\beta lA\omega_0^2\,|\,i-j\,|\,(\epsilon_{n,k}-\epsilon_{1,0})] , \tag{3.20}$$

where n is a band index and k a wave vector in the reduced-zone scheme, so that $\epsilon_{n,k}$ is as given in (3.12). $|\,n,k\rangle$ denotes a Bloch eigenfunction $u_{n,k}(\phi)e^{ik\phi}$ of the type defined in (3.11), and is normalized to unity over one period:

$$\int_{-p/2}^{p/2}d\phi\,|\,u_{n,k}(\phi)\,|^2=1 . \tag{3.21}$$

The unnormalized matrix element $\langle n',k'\,|\,F(\phi)\,|\,n,k\rangle$ is essentially a Fourier integral transform, and is given by

$$\langle n',k'\,|\,F(\phi)\,|\,n,k\rangle \equiv\int_{-\infty}^{+\infty}d\phi\,u_{n',k'}^*(\phi)e^{-ik'\phi}F(\phi)u_{n,k}(\phi)e^{ik\phi} , \tag{3.22}$$

while the normalized matrix element $\langle n',k'\,|\,F(\phi)\,|\,n,k\rangle_N$ is defined as

$$\langle n',k'\,|\,F(\phi)\,|\,n,k\rangle_N =\lim_{M\to\infty}\frac{1}{M}\int_{-Mp/2}^{Mp/2}u_{n',k'}^*(\phi)e^{-ik'\phi}F(\phi) \times u_{n,k}(\phi)e^{ik\phi} . \tag{3.23}$$

The normalized matrix element is thus a finite function of k and k' for any reasonably behaved function $F(\phi)$ that does not diverge at $\phi=\pm\infty$, while the unnormalized matrix element, if $F(\phi)$ itself goes as $\exp(iq_F\phi)$, would give a result proportional to $\delta(q_F+k-k')$ (Bragg diffraction condition in one dimension). Below it will be seen that this is in fact the case for the functions $F_{\rm I}(\phi)$ and $F_{\rm II}(\phi)$ sensitive to the type-I and -II kinks, respectively. The choice of the forms of the $F_i(\phi)$ that are kink-sensitive is in spirit a phenomenological matter, and is therefore deferred to the end of Sec. IV. Appropriate $F_i(\phi)$ will be defined and substituted into (3.20); we will then find the same quantity phenomenologically, and compare the two results. First, though, we find the phenomenological free energy and compare it with its exact counterpart computed above.

IV. PHENOMENOLOGY

Some time ago, Krumhansl and Schrieffer[1] (KS) developed a phenomenological means for the computation of the free energy of a soliton-bearing system; in their model they attempted to obtain, for a ϕ^4 on-site potential, the phonon plus tunneling terms in (3.7) by assuming two noninteracting ideal gases, one composed of relativistic particles (the kinks), and the other of phonons. Their result for the free energy of the soliton gas agreed with that given by the transfer-integral method to within a slowly varying temperature-dependent factor.

CKBT (Ref. 2) improved on the model of KS by taking into account the interaction between kinks and phonons analyzed in Sec. II; our paper follows their treatment. They compute that part, Σ, of the free energy due to the interaction of the phonon gas with one stationary solitonic excitation [kink or antikink; see remark following Eq. (2.16)]. Σ is itself the sum of two terms: (i) ΔF, which is the change in free energy of the extended phonons due to the presence of a kink, and (ii) $F_{\rm int}$, which is the total free energy of any internal modes of oscillation [excited bound states of $V''(\phi_{\pm}^{(0)}(x))$] the kink may possess. CKBT assume that the free energy due to the kink-phonon interaction in the presence of a total of r noninteracting solitonic excitations is simply $r\Sigma$; the thermodynamics for the system is then computed via a model of an ideal gas of kinks plus their associated phonons in which the influence of the kinks on the phonons is incorporated by renormalizing the rest energy of each kink particle from $E^{(0)}$ to $E^{(0)}+\Sigma$. This renormalized kink-gas model precisely reproduces the tunneling component in the transfer-integral free energy for a wide class of systems supporting one type of soliton[2,9]; in all cases for which calculations have been carried to completion, the agreement is numerically exact[2,9] at low temperatures.

Below it is shown that the natural extension to doubly periodic systems of the CKBT theory meets with success. In this generalization, we simply renormalize the rest energy of the ith type of kink ($i={\rm I,II}$) by that amount of free energy Σ_i due to the influence of an isolated kink of that type on the phonons; the only complication in the analysis is a combinatorial argument needed to comply with the topological features of doubly periodic potentials that restrict the possible sequential arrangements of the two types of kinks and antikinks. [This same combinatorial restriction also applies, in simplified form, to monokink systems; when invoked for those potentials (given in Refs. 2 and 5) for which low-temperature exact and phenomenological results can be explicitly compared, it improves upon earlier results by giving exact numerical agreement for all such potentials.]

The kink self- (free) energy Σ_i has the form[2]

$$\Sigma_i=\Delta F_i+k_BT\sum_{n=2}^{N_b^i}\ln(\beta\hbar\omega_{i,n})\ , \tag{4.1}$$

where ΔF_i is the change in the free energy of spatially extended small oscillations due to the presence of a slowly moving kink of type i, and the second term is the classical free energy of small oscillations (if any) localized about the center of the kink [N_b^i is the total number of bound states of the scattering potential (2.16) for the ith type of kink]. The quantities ΔF_i can be expressed,[9] via the change in the phonon density of states,[2] in terms of the phase shift functions $\Delta_i^{\pm}(k)$ introduced in Sec. II:

$$\Delta F_i=-k_BTN_b^i\ln(\beta\hbar\omega_0)$$
$$-\frac{k_BT}{4\pi}\int_{-\infty}^{+\infty}\frac{dk}{k+i}[\Delta_i^+(k)+\Delta_i^-(k)]\ , \tag{4.2}$$

where the i ($=\sqrt{-1}$) appearing in the denominator of the integrand is not to be confused with the kink-type label. With the use of the analytic properties of the phase shifts it is possible to perform[9] the integration over k in Eq. (4.2) without explicit knowledge of these phase shifts. We obtain[9] the result

$$\Sigma_i=-k_BT\ln(\beta\hbar\omega_0)+\zeta_i\quad(i={\rm I,II})\ , \tag{4.3}$$

where the temperature-independent quantities ζ_i are

given by

$$\zeta_{\rm I}=\ln[2^{-1/4}(\mathscr{A}^{\rm I})^{-1/2}\phi_1 e^{\eta_{\rm I}}] \tag{4.4a}$$

and

$$\zeta_{\rm II}=\ln[2^{-1/4}(\mathscr{A}^{\rm II})^{-1/2}(\tfrac{1}{2}p-\phi_1)e^{\eta_{\rm II}}] \ . \tag{4.4b}$$

The quantities $\mathscr{A}^i$ and η_i are directly related to the local potential via Eqs. (1.3) and (3.10), respectively.

We now consider the statistical mechanics of a topologically restricted ideal gas consisting of two types of particles (type I and type II kinks) with renormalized energies given by the nonrelativistic approximation valid at low temperatures ($k_BT \ll E_i^{(0)}$):

$$E_i(p)\cong E_i^{(0)}+\Sigma_i+\frac{p_i}{2M_i} \ . \tag{4.5}$$

In contrast to previous work,[2,5] in which kinks and antikinks were treated as separate particles, we regard a type-i kink and a type-i antikink to be different states of the same particle; kinks and antikinks will be taken to occupy different sectors of phase space denoted by "plus" and "minus," respectively. This concept is illustrated in Fig. 9; the dots represent the locations of kink excitations of the types denoted by the corresponding numerals (I or II), and the two ordered sets of plus and minus signs below the dots give the only two possible arrangements of kinks and antikinks for this particular configuration of type-I and type-II excitations. These restrictions follow from the basic form of a doubly periodic potential given in Fig. 3. Starting our analysis at the right of the line of dots in Fig. 9, we have a type-II followed by a type-I excitation as we move to the left. If the type II is a kink, then between the type-II and type-I kinks the ϕ field is in a well centered at $np-\phi_1$, so that the type-I excitation must also be a kink; similarly, the type I must be an antikink if the type II is an antikink. Consideration of other cases gives for doubly periodic topology the following general rule: Adjacent solitons of the same type occupy opposite sectors of phase space, while adjacent solitons of opposite type occupy the same sector. The sectors occupied by all $N_{\rm I}+N_{\rm II}$ excitations are therefore determined by (1) the locations of the $N_{\rm I}$ points occupied by type-I solitons, (2) the locations of the $N_{\rm II}$ points occupied by type-II solitons, and (3) the sector occupied by any one of the $N_{\rm I}+N_{\rm II}$ solitons. The restrictive role of the topology is thus to reduce from $2^{N_{\rm I}+N_{\rm II}}$ to 2 the possible states in "sector space" corresponding to a given set of $N_{\rm I}$ sites occupied by the type-I particles and $N_{\rm II}$ by the type-II particles.

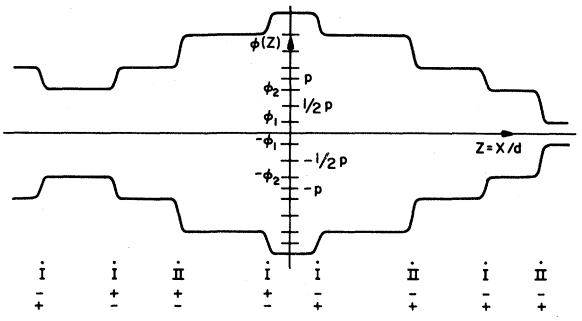

FIG. 9. Topological restrictions of a doubly periodic local potential. Shown are the two possible configurations compatible with a given sequence of type-I and type-II excitations. The dots specify the positions of the excitations; the plus and minus signs denote kinks and antikinks, respectively.

All values of $N_{\rm I}$ and $N_{\rm II}$ are possible for a doubly periodic system. We therefore obtain the thermodynamic functions from the grand canonical kink partition function Ξ_K, which is given by

$$\Xi_K=\sum_{N_I=0}^{\infty}\sum_{N_{\rm II}=0}^{\infty}\exp(\beta\mu_{\rm I}N_{\rm I})\exp(\beta\mu_{\rm II}N_{\rm II}) \times Z(N_{\rm I},N_{\rm II}) \ , \tag{4.6}$$

where $\mu_{\rm I}$ and $\mu_{\rm II}$ are chemical potentials for the two types of solitons, and $Z(N_{\rm I},N_{\rm II})$ is the canonical partition function for a system of length L that supports $N_{\rm I}$ type-I excitations and $N_{\rm II}$ type-II excitations:

$$Z(N_{\rm I},N_{\rm II})=\frac{2}{h^{(N_{\rm I}+N_{\rm II})}}\int_0^L dq_{N_{\rm I}}\int_0^{q_{N_{\rm I}}} dq_{N_{\rm I}-1}\cdots\int_0^{q_2} dq_1\int_0^L dq'_{N_{\rm II}}\int_0^{q'_{N_{\rm II}}} dq'_{N_{\rm II}-1}\cdots\int_0^{q'_2} dq'_1 \times\prod_{i=1}^{N_{\rm I}}\int_{-\infty}^{+\infty} dp_i\prod_{j=1}^{N_{\rm II}}\int_{-\infty}^{+\infty} dp'_j\exp[-\beta E_{\rm I}(p_i)]\exp[-\beta E_{\rm II}(p'_j)] \ . \tag{4.7}$$

The unprimed and primed variables refer to types I and II, respectively, with the q and q' denoting the centers of kink excitations, while p_i and p'_j denote the particle momenta. The restrictions on the coordinate integrals

arise because "correct Boltzmann" (i.e., quantum[35]) counting requires that all solitons of a given type be regarded as indistinguishable. We are thus in effect summing over different states, or configurations, just as in the transfer-integral method; a state is characterized only by the positions of the soliton centers, not by the arbitrary labels attached to these positions. Equation (4.7) also reflects the fact that the energy "state" depends only on the soliton momenta, not on the coordinates or sectors occupied; the prefactor 2 accounts for the twofold degeneracy (kink and antikink) in sector space of each set of momenta and coordinates.

The decoupled momentum integrations are easily carried out to yield

$$\frac{1}{h}\int_{-\infty}^{+\infty} dp \exp[-\beta E_i(p)] = \frac{e^{\xi_i}}{\sqrt{2\pi}}\frac{1}{d}(\beta E_i^{(0)})^{1/2}\exp(-\beta E_i^{(0)}) . \tag{4.8}$$

The restrictions on the coordinate integrals then give

$$Z(N_{\rm I},N_{\rm II}) = 2\left[\frac{1}{N_{\rm I}!}\right]\left[\frac{e^{\xi_{\rm I}}}{\sqrt{2\pi}}\frac{L}{d}(\beta E_{\rm I}^{(0)})^{1/2}\exp(-\beta E_{\rm I}^{(0)})\right]^{N_{\rm I}}\left[\frac{1}{N_{\rm II}!}\right]\left[\frac{e^{\xi_{\rm II}}}{\sqrt{2\pi}}\frac{L}{d}(\beta E_{\rm II}^{(0)})^{1/2}\exp(-\beta E_{\rm II}^{(0)})\right]^{N_{\rm II}} , \tag{4.9}$$

whence

$$\Xi_K = 2\exp\left[\frac{1}{\sqrt{2\pi}}\frac{L}{d}\{e^{\xi_{\rm I}}(\beta E_{\rm I}^{(0)})^{1/2}\exp[-\beta(E_{\rm I}^{(0)}-\mu_{\rm I})]+e^{\xi_{\rm II}}(\beta E_{\rm II}^{(0)})^{1/2}\exp[-\beta(E_{\rm II}^{(0)}-\mu_{\rm II})]\}\right] . \tag{4.10}$$

The form above strongly suggests an alternative derivation of Ξ_K; this other method is worth presenting, because it deals with the topological restrictions from a more local, kink-by-kink picture, thus providing insight into the doubly periodic topology from another viewpoint. Moreover, because this method provides a formalism to label explicitly each excitation's sector, it is preferable for handling systems with a net "winding number" density of kinks over antikinks (or vice versa).[4,6,36]

This alternative method is indicated when Ξ_K from Eq. (4.10) is reexpressed as

$$\Xi_K = 2\sum_{N=0}^{\infty}\frac{1}{N!}\frac{1}{\sqrt{2\pi}}\frac{L}{d}\{e^{\xi_{\rm I}}(\beta E_{\rm I}^{(0)})^{1/2}\exp[-\beta(E_{\rm I}^{(0)}-\mu_{\rm I})]+e^{\xi_{\rm II}}(\beta E_{\rm II}^{(0)})^{1/2}\exp[-\beta(E_{\rm II}^{(0)}-\mu_{\rm II})]\}^N$$

$$=2\sum_{N=0}^{\infty}\frac{1}{h^N}\left[\int_0^L dq_N\prod_{i=1}^{N-1}\int_0^{q_{N-i+1}} dq_{N-i}\right]\prod_{j=1}^{N}\int_{-\infty}^{+\infty} dp_j(\exp\{-\beta[E_{\rm I}(p_j)-\mu_{\rm I}]\}$$

$$+\exp\{-\beta[E_{\rm II}(p_j)-\mu_{\rm II}]\}) . \tag{4.11}$$

The intuitive motivation for the form (4.11) is as follows. The Nth term in the sum accounts for all configurations in which a total of N kinks (plus antikinks), each of which may be either type I or type II, are present on the chain. The prefactor 2 outside the sum indicates that, at the left end point $x=0$, the field can start off in either of two types of wells. These are (option 1) a type-A well with minimum at $\phi=\phi_1+np$, $n=0,\pm1,\pm2,\ldots$, or (option 2) a type-B well with minimum at $\phi=-\phi_1+np$, $n=0,\pm1,\pm2,\ldots$. We first consider option 1, and assume for simplicity that $\phi(x=0)\cong\phi_1$; then the first kink encountered as one moves to the right is identified by the subscript $j=1$ in Eq. (4.11) and can be either a type-I antikink (which evolves the field to the well at $-\phi_1$) or a type-II kink (which evolves the field to the well at $p-\phi_1$). This topologically restricted twofold possibility is expressed by the factor

$$\exp\{-\beta[E_{\rm I}(p_1)-\mu_{\rm I}]\}+\exp\{\beta[E_{\rm II}(p_{\rm I})-\mu_{\rm II}]\}$$

in Eq. (4.11), which acts as a "local partition function" for the site (kink position) indexed by $j=1$.

If one now moves once more to the right until the second kink, with subscript $j=2$, is reached, one

finds that this second excitation can be either a type-I kink or a type-II antikink, regardless of the "choice" made for the $j=1$ particle, since the wells at $\phi=-\phi_1$ and at $\phi=p-\phi_1$ are both type-B wells. As above, this fact is expressed by the "local partition function"

$$\exp\{-\beta[E_{\rm I}(p_2)-\mu_{\rm I}]\}+\exp\{-\beta[E_{\rm II}(p_2)-\mu_{\rm II}]\},$$

and the field will now have been evolved into a type-A well.

One can continue in this manner, moving from left to right until all N excitations in the chain have been accounted for, assigning an integral "site index" j, increasing from 1 to N, to each point q_j at which a kink (or antikink) is centered. Each site will supply another factor

$$\exp\{-\beta[E_{\rm I}(p_j)-\mu_{\rm I}]\}+\exp\{-\beta[E_{\rm II}(p_j)-\mu_{\rm II}]\}$$

to the product in Eq. (4.11). All these factors have identical form, because in the present situation, with the lack of a net winding number density, it is unnecessary to keep track of the sectors occupied by the solitons. However, the above method of counting does provide a means of keeping track should the need arise; specifically, the fact that any kink evolves the system from a type-A well to a type-B well (or vice versa) means that, in option 1, all odd-indexed sites support either a type-I antikink or a type-II kink, while all even-indexed sites support either a type-I kink or a type-II antikink. When combined with the results of a similar analysis for the boundary condition of option 2, this treatment thus provides us with an alternative, local view of the topological restrictions, and especially furnishes a convenient means for generalization of the phenomenology to systems with an externally imposed winding number density. We plan to consider this case further in a future paper.

With the result (4.10) for Ξ_K thus motivated from two different standpoints, we now use it to obtain some thermodynamic quantities of interest for doubly periodic systems. The grand canonical kink potential density $\Omega\equiv-(k_BT/L)\ln\Xi_K$ is given, in the thermodynamic limit $L\to\infty$, by

$$\Omega_K=-\frac{1}{\sqrt{\pi}}\frac{A\omega_0c_0}{d}\left[\frac{k_BT}{A\omega_0c_0}\right]^{1/2}\times\{\phi_1e^{\eta_{\rm I}}\exp[-\beta(E_{\rm I}^{(0)}-\mu_{\rm I})]+(\tfrac{1}{2}p-\phi_1)e^{\eta_{\rm II}}\times\exp[-\beta(E_{\rm II}^{(0)}-\mu_{\rm II})]\}, \quad (4.12)$$

where we have made use of Eqs. (3.5) and (4.4).

Because the renormalization of kink energies[2,5] and all topological restrictions have been accounted for in the partition function $Z(N_{\rm I},N_{\rm II})$, the chemical potentials $\mu_{\rm I}$ and $\mu_{\rm II}$ are set equal to zero after explicit formulas for the average total kink densities (kinks plus antikinks) $n_{\rm I}$ and $n_{\rm II}$ have been obtained:

$$n_{\rm I}=-\left[\frac{\partial\Omega_K}{\partial\mu_{\rm I}}\right]_{\mu_{\rm I}=0}=\frac{\phi_1e^{\eta_{\rm I}}}{\sqrt{\pi}d}\left[\frac{A\omega_0c_0}{k_BT}\right]^{1/2}\times\exp(-\beta E_{\rm I}^{(0)}). \quad (4.13a)$$

and

$$n_{\rm II}=-\left[\frac{\partial\Omega_K}{\partial\mu_{\rm II}}\right]_{\mu_{\rm II}=0}=\frac{\frac{1}{2}p-\phi_1}{\sqrt{\pi}d}e^{\eta_{\rm II}}\left[\frac{A\omega_0c_0}{k_BT}\right]^{1/2}\times\exp(-\beta E_{\rm II}^{(0)}). \quad (4.13b)$$

Then the free-energy density $f_K\equiv\Omega_K+\mu_{\rm I}n_{\rm I}+\mu_{\rm II}n_{\rm II}$ is just

$$f_K=\Omega_K=-k_BT(n_{\rm I}+n_{\rm II}). \quad (4.14)$$

If we compare Eq. (4.14) [using (4.13a) and (4.13b)] with Eq. (3.8) we see that the tunneling portion of the exact, low-temperature, free-energy density is *precisely* reproduced by the kink contributions calculated in a phenomenological ideal-gas picture.

Equations (4.13) hold for *any* doubly periodic potential in the general class described in Sec. I, and in particular we have the following formulas for the kink densities in our two examples: for DPQ,

$$n_{\rm I}=\frac{1}{\sqrt{\pi}d}\left[\frac{A\omega_0c_0}{k_BT}\right]^{1/2}e^{-\beta E_{\rm I}^{(0)}}, \quad (4.15a)$$

$$n_{\rm II}=\frac{\phi_0-1}{\sqrt{\pi}d}\left[\frac{A\omega_0c_0}{k_BT}\right]^{1/2}e^{-\beta E_{\rm II}^{(0)}}, \quad (4.15b)$$

and for DSG,

$$n_i=\frac{(1-\alpha^2)^{1/2}}{\sqrt{\pi}d}\left[\frac{A\omega_0c_0}{k_BT}\right]^{1/2}e^{-\beta E_i^{(0)}},\quad i={\rm I,II}. \quad (4.16)$$

We note that although we did not know the analytic expression for the frequency of the internal mode of the type-I DSG kink (i.e., we only had the numerical result in Fig. 6), it proved unnecessary to have this knowledge for the purpose of obtaining the

kink density. Likewise, it was unnecessary to have explicit expressions for the phase-shift functions $\Delta^{\pm}(k)$. This is a general feature[9] of the ideal-gas phenomenology and has the practical consequence that the kink densities can be found via Eqs. (4.13), which depend only on quantities obtainable *directly* from the local potential $(E_i^{(0)},\eta_i)$. Explicit knowledge of the kink waveforms or their small oscillations is not needed.[9]

The kink contributions to the other thermodynamic functions follow straightforwardly from Eqs. (4.13) and (4.14). For example, the internal energy density is given by

$$u = l^{-1}(k_BT)+n_{\rm I}(E_{\rm I}^{(0)}-\tfrac{1}{2}k_BT) +n_{\rm II}(E_{\rm II}^{(0)}-\tfrac{1}{2}k_BT)\ , \tag{4.17}$$

or, more suggestively,

$$u=\frac{1}{L}\left[\left[\frac{L}{l}-N_b^{\rm I}N_{\rm I}-N_b^{\rm II}N_{\rm II}\right]k_BT +N_{\rm I}[E_{\rm I}^{(0)}+\tfrac{1}{2}k_BT+(N_b^{\rm I}-1)k_BT] + N_{\rm II}[E_{\rm II}^{(0)}+\tfrac{1}{2}k_BT+(N_b^{\rm II}-1)k_BT]\right]. \tag{4.18}$$

$N_i\equiv n_iL$ is the total number of type-i solitons in the system. Equation (4.18) shows u to be simply the internal energy of a system with $L/l-N_b^{\rm I}N_{\rm I}-N_b^{\rm II}N_{II}$ classical phonon modes, and two types of nonrelativistic particles. There are N_i particles of type i; each such particle has rest energy $E_i^{(0)}$, translational energy $\frac{1}{2}k_BT$, and thermal energy k_BT for each of N_b^i-1 internal oscillation modes. Equation (4.18) is thus the natural generalization of the results already found for monokink systems,[2] in that it shows that the type-I and type-II kinks obtain their necessary degrees of freedom at the expense of precisely the correct number of degrees of freedom in the phonon modes.

We now discuss the construction of kink-sensitive functions $F_i(\phi)$ whose correlations [Eq. (3.20)] are characterized by correlation lengths dependent only on the density of kinks of a given type. We note that in the very-low-temperature regime under consideration, the mean square displacement of any mass point due to phonons will be so small that, to zeroth order, the following simple situation prevails: Except for the exponentially small number of lattice sites within those transition regions $\sim d$ over which kinks evolve the field from one minimum to another, every mass point is essentially at some minimum in the potential. The length over which displacements are correlated is thus determined by the kink density,[1,2] the presence of kinks between two points being the only cause for a significant difference in the displacements of those points.

We illustrate the behavior of the kink-detecting functions $F_{\rm I}(\phi)$ and $F_{\rm II}(\phi)$ by looking in detail at the construction of the former of these; for this function $F_{\rm I}(\phi)$, we require that the product $F_{\rm I}(\phi_j)F_{\rm I}(\phi_m)$ of its values at two lattice sites is sensitive to type-I kinks between the jth and mth sites, but totally insensitive to any type-II kinks in this same region of the chain. A straightforward means to this end is to construct $F_{\rm I}(\phi)$ so that it possesses the following properties:

$$F_{\rm I}(-\phi)=-F_{\rm I}(\phi)\ , \tag{4.19a}$$

$$F_{\rm I}\left[\frac{p}{2}+\left[\phi-\frac{p}{2}\right]\right]=F_{\rm I}\left[\frac{p}{2}-\left[\phi-\frac{p}{2}\right]\right]. \tag{4.19b}$$

Together these imply that

$$F_{\rm I}(\phi+p)=-F_{\rm I}(\phi)\ , \tag{4.20a}$$

so that

$$F_{\rm I}(\phi+2p)=F_{\rm I}(\phi)\ . \tag{4.20b}$$

The value of the product $F_{\rm I}(\phi_j)F_{\rm I}(\phi_m)$ thus changes sign when a type-I kink or antikink is encountered in the segment of chain between sites j and m, but remains invariant whenever a type-II kink or antikink is encountered. [Recall that ϕ_j,ϕ_m are located almost exactly at some minima in $V(\phi)$, and that minima in $V(\phi)$ are distributed symmetrically about the centers of barriers I and II; we of course assume that $F_{\rm I}(\phi)\neq 0$ for these minima.]

In a similar fashion, $F_{\rm II}(\phi)$ should satisfy

$$F_{\rm II}(-\phi)=F_{\rm II}(\phi)\ , \tag{4.21a}$$

$$F_{\rm II}\left[\frac{p}{2}+\left[\phi-\frac{p}{2}\right]\right]=-F_{\rm II}\left[\frac{p}{2}-\left[\phi-\frac{p}{2}\right]\right], \tag{4.21b}$$

so that the periodicity properties are

$$F_{\rm II}(\phi+p)=-F_{\rm II}(\phi) \tag{4.22a}$$

and

$$F_{\rm II}(\phi+2p)=F_{\rm II}(\phi) \tag{4.22b}$$

as before.

The relations (4.19)–(4.22) imply that the most

general forms possible for $F_{\rm I}(\phi)$ and $F_{\rm II}(\phi)$ are Fourier series given by

$$F_{\rm I}(\phi)=\sum_{n=1}^{\infty} a_n \sin\left[\frac{(2n+1)\pi\phi}{p}\right], \tag{4.23}$$

$$F_{\rm II}(\phi)=\sum_{n=1}^{\infty} b_n \cos\left[\frac{(2n+1)\pi\phi}{p}\right], \tag{4.24}$$

In the low-temperature limit being dealt with, the functions $F_{\rm I}(\phi)$ will be evaluated only at the discrete set of ϕ equal to minima in $V(\phi)$, so that it is pointless to retain any higher harmonics in the expansions (4.23) and (4.24), and we are left simply with the choices

$$F_{\rm I}(\phi)=\sin\left[\frac{\pi}{p}\phi\right], \qquad F_{\rm II}(\phi)=\cos\left[\frac{\pi}{p}\phi\right]. \tag{4.25}$$

The correlation in the values of $F_i(\phi)$ at two different sites j and m, denoted as in Eq. (3.20) by $\langle F_i(\phi_j)F_i(\phi_m)\rangle$, can be found both phenomenologically and by means of the transfer-integral expression (3.20). This latter result, for which the formalism is more involved, will be evaluated first.

For $x\equiv|m-j|l\gg d$, a ready generalization of the treatment in Ref. 2 shows that the sum in Eq. (3.20) over all bands n reduces to one term, given by the smallest value of the band index n for which the integral over k is nonzero. For the functions given in Eq. (4.25), these values turn out to be $n=2$ for $F_{\rm I}(\phi)$ and $n=1$ for $F_{\rm II}(\phi)$; this follows upon computation of the unnormalized and normalized matrix elements defined in Eqs. (3.22) and (3.23), whose forms are obtained below.

The eigenfunctions $|n,k\rangle\equiv\psi_{n,k}(\phi)$ appearing in Eqs. (3.22) and (3.23) are given, over the interval $-p/2<\phi<p/2$, for $n=1,2$, by[9]

$$\psi_{n,k}(\phi)=\left[\frac{\sigma}{2\pi}\right]^{1/4}\{\exp[-\sigma(\phi+\phi_1)^2-i\nu(k)]+(-1)^{n+1}\exp[-\sigma(\phi-\phi_1)^2+i\nu(k)]\}, \tag{4.26}$$

where

$$\sigma\equiv\tfrac{1}{2}\beta A\omega_0 c_0 \tag{4.27}$$

and

$$\nu(k)=\tfrac{1}{2}\tan^{-1}\left[\frac{\theta\sin(kp)}{1+\theta\cos(kp)}\right], \tag{4.28}$$

with

$$\theta\equiv\left[\left[\frac{p}{\phi_1}\right]-1\right]\exp(\eta_{\rm II}-\eta_{\rm I})\times\exp[-\beta(E_{\rm II}^{(0)}-E_{\rm I}^{(0)})]<1. \tag{4.29}$$

The inequality in Eq. (4.29) follows for reasonably different kink energies, with the η_i defined in Eq. (3.10). $\psi_{n,k}(\phi)$ can then be found for all ϕ from the Bloch relation

$$\psi_{n,k}(\phi+jp)=e^{ijkp}\psi_{n,k}(\phi) \tag{4.30}$$

for any integer j.

The normalized and unnormalized matrix elements involving $F_{\rm I}(\phi)=\sin[(\pi/p)\phi]$ and $F_{\rm II}(\phi)=\cos[(\pi/p)\phi]$ are found by considering expressions of the form

$$\left\langle 1,0\left|\exp\left[\pm\frac{i\pi}{p}\phi\right]\right|n,k\right\rangle,$$

$$\left\langle n,k\left|\exp\left[\pm\frac{i\pi}{p}\phi\right]\right|1,0\right\rangle_N.$$

For example, in the case of

$$\left\langle 1,0\left|\exp\left[\frac{i\pi}{p}\phi\right]\right|1,k\right\rangle,$$

one obtains

$$\left\langle 1,0\left|\exp\left[\frac{i\pi\phi}{p}\right]\right|1,k\right\rangle = \tfrac{1}{2}\left\{\exp\left[-i\left[\nu(k)+\frac{\pi\phi_1}{p}\right]\right]+\exp\left[i\left[\nu(k)+\frac{\pi\phi_1}{p}\right]\right]\right\}\times\sum_{m=-\infty}^{\infty}\exp\left[imp\left[k+\frac{\pi}{p}\right]\right]. \tag{4.31}$$

Since

$$\sum_{m=-\infty}^{\infty}\exp\left[imp\left[k+\frac{\pi}{p}\right]\right]=\sum_{m=-\infty}^{\infty}\exp\left[imp\left[k-\frac{\pi}{p}\right]\right]=\frac{2\pi}{p}\delta\left[k-\frac{\pi}{p}\right], \tag{4.32}$$

we have

$$\left\langle 1,0\left|\exp\left[\frac{i\pi}{p}\phi\right]\right|1,k\right\rangle$$
$$=\frac{2\pi}{p}\delta\left[k-\frac{\pi}{p}\right]\cos\left[\nu(k)+\frac{\pi}{p}\phi_1\right]$$
$$=\frac{2\pi}{p}\delta\left[k-\frac{\pi}{p}\right]\cos\left[\frac{\pi}{p}\phi_1\right], \tag{4.33}$$

where we have used $\nu(k=\pi/p)=0$ from (4.28). The Bloch relation (4.30) indicates that any matrix element

$$\left\langle 1,0\left|\exp\left[\pm\frac{i\pi\phi}{p}\right]\right|n,k\right\rangle$$

is zero unless $k=\pi/p$, so that the "phase difference" $2\nu(k)$ between "atomic" states on the same "dimer" is always zero, and therefore never complicates the analysis.

In addition to the fact that

$$\left\langle n,k\left|\exp\left[\pm\frac{i\pi\phi}{p}\right]\right|1,0\right\rangle_N=0$$

for $k\neq\pi/p$, the delta function in the expression (4.33) for the ordinary matrix element, along with Eq. (3.20), shows that

$$\left\langle n,k=\frac{\pi}{p}\left|F_i(\phi)\right|1,0\right\rangle_N$$

is the only normalized element which enters these correlation functions. By inspection,

$$\left\langle 1,k=\frac{\pi}{p}\left|\exp\left[\frac{i\pi\phi}{p}\right]\right|1,0\right\rangle_N=\cos\left[\frac{\pi\phi_1}{p}\right]. \tag{4.34}$$

When all relevant matrix elements are evaluated, one finds, for $n=1,2$,

$$\langle 1,0\,|\,F_{\rm I}(\phi)\,|\,n,k\rangle$$
$$=-[1+(-1)^n]\frac{\pi}{p}\delta\left[k-\frac{\pi}{p}\right]\sin\left[\frac{\pi\phi_1}{p}\right], \tag{4.35a}$$

$$\langle 1,0\,|\,F_{\rm II}(\phi)\,|\,n,k\rangle$$
$$=[1-(-1)^n]\frac{\pi}{p}\delta\left[k-\frac{\pi}{p}\right]\cos\left[\frac{\pi\phi_1}{p}\right], \tag{4.35b}$$

$$\left\langle n,k=\frac{\pi}{p}\left|F_{\rm I}(\phi)\right|1,0\right\rangle_N$$
$$=-\tfrac{1}{2}[1+(-1)^n]\sin\left[\frac{\pi\phi_1}{p}\right], \tag{4.35c}$$

$$\left\langle n,k=\frac{\pi}{p}\left|F_{\rm II}(\phi)\right|1,0\right\rangle_N$$
$$=\tfrac{1}{2}[1-(-1)^n]\cos\left[\frac{\pi\phi_1}{p}\right]. \tag{4.35d}$$

These formulas clearly exhibit the essential features required for the kink-detecting functions $F_i(\phi)$ mentioned earlier, such as (i) the delta function in the ordinary matrix elements, and (ii) the fact that $F_{\rm I}(\phi)$ couples the ground state to the edge of the $n=2$ band, while $F_{\rm II}(\phi)$ couples the ground state to the edge of the lowest ($n=1$) band. The final results in the continuum notation $x\equiv|m-j|l\gg d$ are thus

$$\langle F_{\rm I}(\phi(0))F_{\rm I}(\phi(x))\rangle=\sin^2\left[\frac{\pi}{p}\phi_1\right]\exp\left[-\frac{x}{\xi_{\rm I}}\right] \tag{4.36a}$$

and

$$\langle F_{\rm II}(\phi(0))F_{\rm II}(\phi(x))\rangle=\cos^2\left[\frac{\pi}{p}\phi_1\right]\exp\left[-\frac{x}{\xi_{\rm II}}\right], \tag{4.36b}$$

where the correlation lengths ξ_i are given by

$$\xi_{\rm I}=[\beta A\omega_0^2(\epsilon_{2,k=\pi/p}-\epsilon_{1,k=0})]^{-1},$$
$$\xi_{\rm II}=[\beta A\omega_0^2(\epsilon_{1,k=\pi/p}-\epsilon_{1,k=0})]^{-1}. \tag{4.37}$$

The features of the band structure described by Eq. (3.13), along with the formula (4.13) for the density n_i of the ith type of kink, yield in general

$$\xi_i=\frac{1}{2n_i}. \tag{4.38}$$

Thus the correlation length for a function sensitive to the ith type of soliton is essentially the inverse density of that type of soliton, a very plausible result suggested by a simple phenomenological argument which we explain below.

The treatment follows that of Krumhansl and Schrieffer,[1] who point out that the exponentially small kink densities imply that the probability $P_i(n;x)$ of finding kinks of ith type separated by distance x, is given by the Poisson distribution:

$$P_i(n,x)=\frac{\langle n_i(x)\rangle^n e^{-\langle n_i(x)\rangle}}{n!}\ , \tag{4.39}$$

where $n_i(x)$, the expected number of kinks between the two points, is just

$$n_i(x)=n_i x\ . \tag{4.40}$$

The appropriate correlation functions are then computed by application of the properties (4.19)–(4.22) characterizing the kink-detecting functions $F_i(\phi)$. The essential feature of these defining properties is this: They ensure that, if there are n_i type-i kinks or antikinks between the two points at which $F_i(\phi)$ is evaluated, then the value of the product $F_i(\phi(0))F_i(\phi(x))$ will be $(-1)^{n_i}F_i^2(\phi_1)$, regardless of the number of kinks of different type which are also present. Thus the correlation functions are given by

$$\begin{aligned}\langle F_i(\phi(0))F_i(\phi(x))\rangle &= \sum_{n=0}^{\infty} F_i^2(\phi_1)(-1)^n P_i(n;x) \\ &= F_i^2(\phi_1)e^{-2n_i x}\ ,\end{aligned} \tag{4.41}$$

which yields a correlation length

$$(\xi_i)_{\text{phen}}=\frac{1}{2n_i}\ , \tag{4.42}$$

in precise agreement with the general result (4.36).

V. SUMMARY AND DISCUSSION

In this paper we have modified and generalized the phenomenological ideal-gas theory of Currie, Krumhansl, Bishop, and Trullinger[2] to include doubly periodic local potentials bearing two types of kink solutions. By properly accounting for the topological restrictions in placing kinks and antikinks of the two types on the one-dimensional chain and employing the kink self-energy correction due to its influence on the phonon free energy, we have found that the phenomenology gives results in precise agreement with those obtained by the transfer-operator method at low temperatures. In addition, we obtained a general kink-density formula (4.13) for this entire class of models that depends only on quantities obtainable directly from the local potential and not on specific details of the kink wave form or its small oscillations.

Much remains to be done, however, to extend the above analysis still further. For example, in experimental situations it is not always possible (or convenient) to work at temperatures low enough to ensure the validity of the ideal-gas approximation (low kink density). For this reason it is desirable to extend the CKBT (Ref. 2) theory to higher temperatures where kink-kink interactions and anharmonic phonon corrections become important. Another area of interest is the nonequilibrium transport properties[37,38] of these models since *two* types of kinks can carry physical signatures (e.g., mass, charge, spin, etc.). A correct quantum theory at finite temperatures[39] is also needed for $k_B T \lesssim \hbar\omega_0$. We hope to address these and other questions in the near future.

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[1]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B 11, 3535 (1975).
[2]J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B 22, 477 (1980).
[3]A. R. Bishop, J. A. Krumhansl, and S. E. Trullinger, Physica D 1, 1 (1980).
[4]J. F. Currie, M. B. Fogel, and F. Palmer, Phys. Rev. A 16, 796 (1977).
[5]S. E. Trullinger and R. M. DeLeonardis, Phys. Rev. A 20, 2225 (1979).
[6]Neelam Gupta and Bill Sutherland, Phys. Rev. A 14, 1790 (1979).
[7]R. A. Guyer and M. D. Miller, Phys. Rev. A 17, 1205 (1978).
[8]R. A. Guyer and M. D. Miller, Phys. Rev. A 17, 1771 (1978).
[9]R. M. DeLeonardis, Ph.D. thesis, University of Southern California, 1980 (unpublished); R. M. DeLeonardis and S. E. Trullinger, Phys. Rev. B 22, 4558 (1980).
[10]R. M. DeLeonardis and S. E. Trullinger, Phys. Rev. A 20, 2603 (1979).
[11]R. K. Bullough and P. J. Caudrey, in *Nonlinear Evolu-*

tion Equations Solvable by the Inverse Spectral Transform, edited by F. Calogero (Pitman, London, 1978), pp. 180–224.
[12]K. Maki and P. Kumar, Phys. Rev. B 14, 118 (1976).
[13]K. Maki and P. Kumar, Phys. Rev. B 14, 3920 (1976).
[14]J. Frenkel and T. Kontorowa, J. Phys. (USSR) 1, 137 (1930).
[15]A. R. Bishop, J. Phys. C 11, L329 (1978).
[16]J. Schiefman and P. Kumar, Phys. Scr. 20, 435 (1979).
[17]D. J. Scalapino, M. Sears, and R. A. Ferrell, Phys. Rev. B 6, 3409 (1972).
[18]J. F. Currie, S. E. Trullinger, A. R. Bishop, and J. A. Krumhansl, Phys. Rev. B 15, 5567 (1977).
[19]M. B. Fogel, S. E. Trullinger, A. R. Bishop, and J. A. Krumhansl, Phys. Rev. Lett. 36, 1411 (1976); Phys. Rev. B 15, 1578 (1977).
[20]G. S. Guralnik, C. R. Hagen, and T. W. B. Kibble, in *Advances in Particle Physics,* edited by R. L. Cool and R. E. Marshak (Wiley, New York, 1968), Vol. 2.
[21]Evans M. Harrell, Commun. Math. Phys. 60, 73 (1978).
[22]Evans M. Harrell, Ann. Phys. 119, 351 (1978).
[23]Sydney Goldstein, Proc. R. Soc. Edinburgh T 49, 210 (1929), Sec. III, Eq. (2).
[24]W. H. Furry, Phys. Rev. 71, 360 (1947).
[25]T. Banks, C. M. Bender, and T. T. Wu, Phys. Rev. D 8, 3346 (1973); T. Banks and C. M. Bender, *ibid.* 8, 3366 (1973).
[26]R. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. D 11, 3424 (1975).
[27]H. Neuberger, Phys. Rev. D 17, 498 (1978).
[28]E. Gildener and A. Patrascioiu, Phys. Rev. D 16, 423 (1977).
[29]E. Gildener and A. Patrascioiu, Phys. Rev. D 16, 1802 (1977).
[30]A. Patrascioiu, Phys. Rev. D 17, 2764 (1978).
[31]J. L. Gervais and B. Sakita, Phys. Rev. D 16, 3507 (1977).
[32]H. J. de Vega, J. L. Gervais, and B. Sakita, Nucl. Phys. B 139, 20 (1978).
[33]H. J. de Vega, J. L. Gervais, and B. Sakita, Nucl. Phys. B 143, 125 (1978).
[34]H. J. de Vega, J. L. Gervais, and B. Sakita, Phys. Rev. D 19, 604 (1979).
[35]Kerson Huang, *Statistical Mechanics* (Wiley, New York, 1963), p. 154.
[36]S. E. Trullinger, Phys. Rev. B 22, 418 (1980).
[37]S. E. Trullinger, M. D. Miller, R. A. Guyer, A. R. Bishop, F. Palmer, and J. A. Krumhansl, Phys. Rev. Lett. 40, 206 (1978); 40, 1603(E) (1978).
[38]M. Büttiker and R. Landauer, Phys. Rev. Lett. 43, 1453 (1979).
[39]K. Maki and H. Takayama, Phys. Rev. B 20, 3223 (1979); 20, 5002 (1979); 20, 5009 (1979).