

Low-temperature soliton-gas phenomenology for sine-Gordon systems with a winding-number density

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The ideal-kink-gas phenomenology of Currie, Krumhansl, Bishop, and Trullinger is extended to include the case of nonzero winding-number density in sine-Gordon systems. By considering kinks and antikinks to be substates of a single type of "particle" and taking into account the renormalization of the kink energy due to phase-shift interactions between kinks and phonons, simple expressions are obtained for the low-temperature, average kink and winding-number densities as a function of the winding-number potential. The results agree with the exact transfer-operator results of Currie, Fogel, and Palmer.

I. INTRODUCTION

Recently Currie, Krumhansl, Bishop, and Trullinger¹ (hereafter referred to as CKBT) have formulated an ideal-gas phenomenology for the classical statistical mechanics of one-dimensional kink-bearing systems such as the sine-Gordon (SG) and ϕ -four prototypes. A major ingredient of the work by CKBT was the influence of the kinks on the phonon density of states via phase-shift interactions, leading to a renormalization of the kink creation energy, i.e., a kink self-energy correction. This effect had been neglected in the earlier work by Krumhansl and Schrieffer² on the ϕ -four problem, and its inclusion was shown by CKBT to be absolutely essential in correctly accounting for the various degrees of freedom in the problem. By considering a dilute gas of *renormalized* kinks, CKBT were able to demonstrate the low-temperature equivalence of their phenomenology with exact results obtainable from a transfer-integral approach.

In their work CKBT focused on the simplest situation where periodic boundary conditions are imposed on the field variable: $\phi(L, t) = \phi(0, t)$, where L is the length of the system. In a canonical ensemble this forces the number of kinks to equal the number of antikinks. In a grand canonical ensemble such as the one employed by CKBT, the numbers of kinks and antikinks are not fixed, but nevertheless the equality of kink and antikink energies causes those members of the ensemble with equal numbers of each to dominate the grand canonical partition function. As a consequence the *average* kink and antikink numbers are equal. In several physical situations, however, there may be *external* constraints or forces which dictate an imbalance of kink and antikink numbers. For example, in certain quasi-one-dimensional charge-density-wave (CDW) systems, the CDW wave vector may be incommensurate with

the underlying lattice period,³ and in such cases there is a preference for kinks over antikinks or vice versa. The details of this preference depend on the degree of commensurability⁴ and on whether⁵ a charge reservoir is in contact with the system.

In this paper we extend the CKBT phenomenology to include cases where external constraints are imposed to yield a *net* number of kinks minus antikinks, i.e., a net "winding-number" density.^{6,7} The simplest model system where this can occur is the sine-Gordon system and we treat this case here. More exotic systems, such as "double sine-Gordon"⁸ with two types of kinks (and antikinks), will be treated in a separate publication. We shall assume that the winding-number density $n_w \equiv [\phi(L) - \phi(0)]/2\pi L$, is related to a conjugate "winding-number potential," λ , which plays a role similar to that of a chemical potential.

In Sec. II we review the source and derivation of the kink (soliton) self-energy introduced by CKBT and we extend their analysis to include the velocity dependence of the kink-energy renormalization. In Sec. III, we construct a grand canonical formalism for the calculation of thermodynamic functions. Non-trivial improvements of the CKBT procedure are required when the winding-number density is nonzero. In particular, we shall find it convenient to regard kinks and antikinks as substates of *one* species of "particle." We compare our phenomenological results with those of the exact transfer-operator approach^{6,7} and find *exact* agreement at low temperatures.

II. THE KINK SELF-ENERGY

In the notation used by CKBT the sine-Gordon Hamiltonian is written as

$$H = A \int dx \left[\frac{1}{2} \phi_t^2 + \frac{1}{2} c_0^2 \phi_x^2 + \omega_0^2 (1 - \cos \phi) \right], \quad (2.1)$$

where $\phi(x, t)$ is the dimensionless sine-Gordon (SG) field. The constant c_0 is a characteristic velocity and the constant ω_0 is a characteristic frequency for the system. The overall constant A sets the energy scale and has dimensions of (energy) \times (length) $^{-1}$ \times (time) 2 . The ratio $d \equiv c_0/\omega_0$ serves as a fundamental length scale in the system and provides a measure of the "width" of the kink excitation.

The single-kink solutions to the Euler-Lagrange equation of motion

$$\phi_{tt} - c_0^2 \phi_{xx} + \omega_0^2 \sin \phi = 0 \quad (2.2)$$

have the form

$$\phi^{(\nu)}(x, t) = 4 \tan^{-1} [\exp(+\gamma(x - \nu t)/d)] \quad (2.3)$$

where ν is the velocity of the kink (+) or antikink (-) and $\gamma = (1 - \nu^2/c_0^2)^{-1/2}$. The excess energy E_K , associated with a single kink has the pseudorelativistic form

$$E_K^{(\nu)} = \gamma E_K^{(0)} = (E_K^{(0)2} + p^2 c_0^2)^{1/2} \quad (2.4)$$

where $p = \gamma M_K \nu$ is the "relativistic" momentum and $E_K^{(0)}$ is the rest energy of the kink (antikink) 1

$$E_K^{(0)} = 8A \omega_0 c_0 = M_K c_0^2 \quad (2.5)$$

Here $M_K = 8A \omega_0/c_0$ is the kink rest mass.

As emphasized by CKBT, the presence of a kink in the system influences the density of states for small-amplitude solutions to the linearized equation of motion [$\sin \phi \rightarrow \phi$ in Eq. (2.2)]. The behavior of such small oscillations (phonons) in the presence of a single static kink is determined by finding solutions to Eq. (2.2) of the form

$$\phi(x, t) = \phi_K^{(0)}(x) + \chi(x, t) \quad (2.6)$$

where $\chi(x, t)$ is small. Phonons in the presence of moving kinks can be obtained from those for a static kink by "Lorentz boosting" to the kink rest frame. Substitution of Eq. (2.6) into Eq. (2.2) and linearization in χ gives

$$\chi_{tt} - c_0^2 \chi_{xx} + \omega_0^2 [1 - 2 \operatorname{sech}^2(x/d)] \chi = 0 \quad (2.7)$$

Writing χ as $\chi(x, t) = f(x) e^{-i\omega t}$ leads to the following eigenvalue equation:

$$-c_0^2 f_{xx} + \omega_0^2 [1 - 2 \operatorname{sech}^2(x/d)] f = \omega^2 f \quad (2.8)$$

This has the form of a Schrödinger equation for a "particle" moving in a one-dimensional potential well [$\sim 1 - 2 \operatorname{sech}^2(x/d)$]. The spectrum of solutions 9 to Eq. (2.8) contains exactly *one* "bound state" (the "translation mode" 1)

$$f_b(x) = (2d)^{-1/2} \operatorname{sech}(x/d); \quad \omega_b^2 = 0 \quad (2.9)$$

and the continuum or scattering states 1

$$f_k(x) = (2\pi)^{-1/2} \omega_k^{-1} e^{ikx} [kd + i \tanh(x/d)] \quad (2.10)$$

$$\omega_k^2 = \omega_0^2 + c_0^2 k^2$$

Note that the dispersion relation (2.10) for these continuum states is exactly the same as for phonons in the absence of a kink and, indeed, the waveform $f_k(x)$ approaches that of a pure phonon ($\sim e^{ikx}$) far away from the kink "center" at $x=0$. However, there is a distortion near the kink which results in a "phase shift" of the phonon 1

$$\Delta(k) = \pi \frac{k}{|k|} - 2 \tan^{-1} kd \quad (2.11)$$

For a kink moving with velocity ν , the velocity-dependent phase shift can be obtained from Eq. (2.11) by a Lorentz boost

$$\Delta(k; \nu) = \Delta(\gamma [k - (\nu \omega_0/c_0^2) (1 + k^2 d^2)^{1/2}]; 0) \quad (2.12)$$

We note here that the equations following Eq. (2.6) are insensitive to our choice of either a kink (+) or antikink (-) solution $\phi_K^{(0)}(x)$. Thus, *from the point of view of the phonons, an antikink is indistinguishable from a kink*. This will have important implications in Sec. III when we develop the kink-gas phenomenology.

We now make use of the information contained in $\Delta(k; \nu)$ to examine the effect of kink excitations on the density of states for the phonons. Because the presence of a kink changes this density of states, there is a corresponding change 1 in the phonon free energy when a kink is introduced into the system. This led CKBT to define a "self-energy" for the kink which takes into account the fact that kinks and phonons *share* 1 the available degrees of freedom.

Consider a large system of length L and suppose first that there is one kink (or antikink) at rest at $x=0$. If we impose periodic (Born-von Karman) boundary conditions on the continuum (phonon) state solutions $f_k(x)$ of Eq. (2.8), the allowed wave vectors k are determined by the condition 1

$$Lk_n + \Delta(k_n) = 2\pi n \quad (n=0, \pm 1, \pm 2, \dots) \quad (2.13)$$

The phonon density of states is then

$$\rho(k) = \frac{dn}{dk} = \frac{L}{2\pi} + \frac{1}{2\pi} \frac{d\Delta(k)}{dk} \quad (2.14)$$

In the absence of a kink, the density of states is $\rho_0(k) = L/2\pi$ so that the change is given by

$$\Delta\rho(k) = \rho(k) - \rho_0(k) = \frac{1}{2\pi} \frac{d\Delta(k)}{dk} \quad (2.15)$$

In analogy with the Friedel sum rule 10 (e.g., for impurity states in a metal) there can be *no net* change in the total number of states when the kink is introduced. Since there is one bound-state solution of Eq. (2.8), the total number of extended phonon states must be *decreased* by one; i.e.,

$$\oint dk \Delta\rho(k) = -\frac{1}{\pi} \Delta(0^+) = -1 \quad (2.16)$$

where \mathcal{P} denotes the Cauchy principal value, and we have used the fact that $\lim_{k \rightarrow \infty} \Delta(k) = 0$. Note that Eq. (2.16) also follows from Levinson's theorem¹¹

$$\Delta(0^+) = \pi \mathfrak{N} \quad (2.17)$$

where \mathfrak{N} is the number of bound states.

One way to view¹ this decrease is that the kink (or antikink) "traps" a phonon state due to its very presence. Not only is the trapping of a phonon state unavoidable, it is *precisely* the mechanism by which the kink can divert two degrees of freedom for its creation and translational motion.

In the next section we shall define a grand canonical partition function for the system by considering the excitations to be comprised of kinks and antikinks at low enough densities so that they can be regarded as noninteracting "particles." In order to account properly for the phonon excitations as well, it is essential to remember that the density of states for the phonons *depends* on the kink configuration.

Thus, the phonons are *not* independent of the kinks, but rather must be regarded as being *associated with* the kinks. Because of this association we shall refer to these phonons as "kink phonons," and emphasize that this association *precludes* the factorization of the

partition function into independent kink and phonon pieces. Indeed, *before* we can integrate over kink position and velocity phase-space variables, we *must* integrate over the kink-phonon phase space associated with kinks moving with particular velocities. Only then may we integrate over kink velocities to obtain the kink partition function.

As a preliminary step in calculating this partition function, we therefore require the calculation of the free energy of the kink phonons associated with a particular configuration of N kinks and antikinks moving with velocities $v_j (j = 1, 2, \dots, N)$. For this purpose we use the fact that each kink and antikink contributes *independently* to the change in the phonon density of states, since the phase shifts in the SG case are additive.¹² The total kink-phonon free energy is then written as

$$F_{\text{kink-phonon}} = F_0 + \sum_{j=1}^N \Delta F(v_j) \quad (2.18)$$

where F_0 is the unperturbed phonon free energy in the absence of kinks,¹ and $\Delta F(v)$ is *change*¹ in classical phonon free energy caused by a kink (or antikink) moving with velocity v (in the limit of vanishing lattice constant)

$$\begin{aligned} \Delta F(v) &= k_B T \mathcal{P} \int_{-\infty}^{+\infty} dk \Delta \rho(k; v) \ln(\beta \hbar \omega_k) = \frac{k_B T}{2\pi} \mathcal{P} \int_{-\infty}^{+\infty} dk \frac{d\Delta(k; v)}{dk} \ln[\beta \hbar \omega_0 (1 + k^2 d^2)^{1/2}] \\ &= -k_B T \ln(\beta \hbar \omega_0) + \frac{k_B T}{2\pi} \mathcal{P} \int_{-\infty}^{+\infty} dk \frac{d\Delta(k; v)}{dk} \ln(1 + k^2 d^2)^{1/2} \quad , \beta \equiv (k_B T)^{-1} \quad , \end{aligned} \quad (2.19)$$

where Eq. (2.16) has been used and $\Delta(k; v)$ is the kink-velocity-dependent phonon phase shift given by Eq. (2.12). In performing the integration in Eq. (2.19) it is convenient to transform from k to $k' = \gamma [k - (v\omega_0/c_0^2)(1 + k^2 d^2)^{1/2}]$. We then make use of the relation

$$(1 + k^2 d^2)^{1/2} = \gamma [(1 + k'^2 d^2)^{1/2} + (v/c_0) k' d] \quad (2.20)$$

to write

$$\Delta F(v) = -k_B T \ln(\gamma \beta \hbar \omega_0) + \frac{k_B T}{2\pi} \mathcal{P} \int_{-\infty}^{+\infty} dk' \frac{d\Delta(k')}{dk'} \ln[(1 + k'^2 d^2)^{1/2} + (v/c_0) k' d] \quad (2.21)$$

If we then make use of the fact that $d\Delta/dk'$ is an even function of k' we have

$$\begin{aligned} \Delta F(v) &= -k_B T \ln(\gamma \beta \hbar \omega_0) - \frac{k_B T}{2\pi} d \int_{-\infty}^{+\infty} \frac{dk'}{1 + k'^2 d^2} \ln(1 + \gamma^{-2} k'^2 d^2) = -k_B T \ln(\gamma \beta \hbar \omega_0) - k_B T \ln(1 + \gamma^{-1}) \\ &= -k_B T \ln[(1 + \gamma) \beta \hbar \omega_0] \quad . \end{aligned} \quad (2.22)$$

Since ΔF depends on the velocity v of the kink (or antikink) only through the Lorentz factor $\gamma = (1 - v^2/c_0^2)^{-1/2}$, we see that ΔF is an even function of v , as it should be.

We shall regard the change in phonon free energy due to a kink moving with velocity v as a self-energy of the kink $\sum_K(\gamma) = \Delta F(\gamma)$. As we shall see in the next section, the grand canonical partition function for the system can be obtained by regarding the kinks (and antikinks) as "particles" with "renormalized"

energies

$$\begin{aligned} E_K^*(\gamma) &= \gamma E_K^{(0)} + \sum_K(\gamma) \\ &= \gamma E_K^{(0)} - k_B T \ln[(1 + \gamma) \beta \hbar \omega_0] \quad . \end{aligned} \quad (2.23)$$

III. KINK-GAS PHENOMENOLOGY

In this section we extend and modify the ideal-gas phenomenology developed¹ by CKBT to include the

case of nonzero winding-number density

$$n_w = [\phi(L) - \phi(0)]/2\pi L \quad (3.1)$$

We restrict ourselves to the case where the total number of kinks (including antikinks) is low so that we may ignore interactions between them.¹ The winding-number density (3.1) may then be re-expressed in terms of the difference of kink and antikink number densities

$$n_w = (N_K - N_{\bar{K}})/L = n_K - n_{\bar{K}} \quad (3.2)$$

since these are the only stable excitations which can evolve the field between the degenerate wells in the SG potential $(1 - \cos\phi)$.

There are two basic ways in which to view a nonzero value of n_w . It may arise by a direct constraint (such as the introduction of a fixed amount of excess charge in a CDW system), or it may arise because of a winding-number potential λ which causes a *tendency* for n_w to be nonzero but does not *preclude* fluctuations in the winding number. We shall consider the latter situation here since it is the more general case. By using what amounts to a grand canonical ensemble with a partition function that is λ dependent, we can, in fact, obtain results which are valid for the former case (fixed n_w) as well, in the same way that the ordinary grand canonical ensemble can be used to obtain results for systems with a fixed number of particles. In other words, if λ is the quantity which is fixed externally, we can determine $\langle n_w \rangle$ as a function of λ ; if n_w is fixed externally we can choose λ so that $\langle n_w \rangle = n_w$.

We regard the system as an ideal gas of kinks (including antikinks) and their attendant kink phonons. Before we can integrate over kink momenta, we must first integrate over the kink-phonon degrees of freedom, since these *depend* on the kink velocities. This has already been accomplished in Sec. II where we saw that the influence of the kinks on the phonon free energy could be accounted for in terms of "self-energies" \sum_K for the kinks. We now therefore write the grand canonical partition function $\Xi(T, L, \mu, \lambda)$

$$Z_N^*(T, L, \lambda) = \frac{1}{h^N} \int_0^L dq_1 \int_0^{q_1} dq_2 \cdots \int_0^{q_{N-1}} dq_N \int_{-\infty}^{+\infty} dp_1 \cdots \int_{-\infty}^{+\infty} dp_N \prod_{j=1}^N \left[e^{-\beta E_K^*(p_j)} \sum_{\sigma_j = \pm 1} e^{\beta \lambda \sigma_j} \right] \quad (3.6)$$

The limits on the q integrations take into account the correct "Boltzmann counting" (indistinguishable nature of truly "quantum" particles). Note that the winding-number potential λ favors kinks ($\sigma = +1$) over antikinks ($\sigma = -1$) if $\lambda > 0$ and vice versa if $\lambda < 0$. Upon carrying out the q integrations and the σ summations, Z_N^* may be rewritten as

$$Z_N^*(T, L, \lambda) = \frac{1}{N!} \left[\frac{2L}{h} \cosh \beta \lambda \int_{-\infty}^{+\infty} dp e^{-E_K^*(p)} \right]^N = \frac{1}{N!} z^N \quad (3.7)$$

for the system as

$$\Xi(T, L, \mu, \lambda) \cong e^{-\beta F_0} \Xi_K^*(T, L, \mu, \lambda) \quad (3.3)$$

where F_0 is the zero-kink phonon free energy and

$$\Xi_K^*(T, L, \mu, \lambda) = \sum_{N=0}^{\infty} e^{\beta \mu N} Z_N^*(T, L, \lambda) \quad (3.4)$$

is a grand canonical partition function for renormalized kinks (including antikinks). Here Z_N^* is the partition function for a system of N renormalized kinks, where N refers to the *total* number of kinks *plus* antikinks. Indeed, there is no reference to whether a "particle" is a kink or an antikink, since *both* possibilities will be summed over in calculating Z_N^* . In other words, the kink and antikink excitations are regarded as substates of the same particle. This is in contrast to the approach of CKBT,¹ who regard kinks and antikinks as *separate* ideal gases. While their approach can be used when $n_w = 0$, it fails when $n_w \neq 0$ since the number of kinks is *not* independent of the number of antikinks in this latter case.

The sole purpose of introducing the chemical potential μ in Ξ_K^* is to allow a convenient and self-consistent definition of the average total kink density (including antikinks)

$$\langle n_{\text{tot}} \rangle = \frac{\langle N \rangle}{L} = \frac{1}{\beta L} \left[\frac{\partial}{\partial \mu} \ln \Xi_K^*(T, L, \mu, \lambda) \right]_{\mu=0} \quad (3.5)$$

In this expression we set $\mu = 0$ after performing the derivative since we have already accounted for the kink self-energy due to its effect on the phonons; the *renormalized* energy E_K^* will be used in calculating Z_N^* . The total kink density depends only on the temperature T and winding-number potential λ ; thus in the same way that the photon or phonon gas has $\mu = 0$, we must also require $\mu = 0$.

We now calculate the N -kink partition function $Z_N^*(T, L, \lambda)$. This is done by considering N particles placed along a line at positions q_1, q_2, \dots, q_N , with momenta p_1, p_2, \dots, p_N and integrating over q and p and summing over a kink-antikink index σ

where z is the single-particle partition function

$$z = \frac{2L}{h} \cosh \beta \lambda \int_{-\infty}^{+\infty} dp e^{-\beta E_K^*(p)} \quad (3.8)$$

To evaluate z we change variables from p to γ

$$z = \frac{4L}{h} (\cosh \beta \lambda) M_K c_0 \int_1^{\infty} \frac{d\gamma \gamma}{(\gamma^2 - 1)^{1/2}} e^{-\beta E_K^*(\gamma)} \quad (3.9)$$

where $E_K^*(\gamma)$ is given by Eq. (2.23). If we define the quantities

$$\gamma \equiv \gamma - 1, \quad \eta \equiv \beta E_K^{(0)} \quad (3.10)$$

and use Eq. (2.23), z can be rewritten as

$$z = \frac{2L}{\pi d} (\cosh\beta\lambda) \eta e^{-\eta} \left(\frac{\partial^2}{\partial \eta^2} - 3 \frac{\partial}{\partial \eta} + 2 \right) \int_0^\infty \frac{dy}{\sqrt{y(y+2)}} e^{-\eta y} . \quad (3.11)$$

The integral appearing in Eq. (3.11) can be found in tables¹³

$$\int_0^\infty \frac{dy}{\sqrt{y(y+2)}} e^{-\eta y} = e^\eta K_0(\eta) , \quad (3.12)$$

where $K_0(\eta)$ is the modified Bessel function.¹⁴ Thus,

$$z = \frac{2L}{\pi d} \cosh\beta\lambda \{ \beta E_K^{(0)} [K_0(\beta E_K^{(0)}) + K_1(\beta E_K^{(0)})] + K_1(\beta E_K^{(0)}) \} . \quad (3.13)$$

In order for the kink density to be low so that our noninteracting gas approximation is valid, we must restrict ourselves to the low-temperature region $k_B T \ll E_K^{(0)}$ ($\beta E_K^{(0)} \gg 1$). Using the asymptotic forms¹⁴ of the Bessel functions, we find:

$$z \cong \left(\frac{2}{\pi} \right)^{1/2} \frac{2L}{d} (\cosh\beta\lambda) (\beta E_K^{(0)})^{1/2} \left[1 + \frac{5}{8} (\beta E_K^{(0)})^{-1} + \frac{21}{128} (\beta E_K^{(0)})^{-2} + \dots \right] e^{-\beta E_K^{(0)}} , \quad \beta E_K^{(0)} \gg 1 . \quad (3.14)$$

Now that we have an explicit expression for the single-particle partition function z we may calculate all thermodynamic quantities of interest. The grand canonical kink partition function is obtained from Eqs. (3.4) and (3.7)

$$\Xi_K^*(T, L, \mu, \lambda) = \sum_{N=0}^{\infty} \frac{e^{\beta \mu N} z^N}{N!} = \exp(z e^{\beta \mu}) . \quad (3.15)$$

The average total kink density is given according to Eq. (3.5) as

$$\langle n_{\text{tot}} \rangle = z/L \cong \left(\frac{2}{\pi} \right)^{1/2} \frac{2}{d} (\cosh\beta\lambda) (\beta E_K^{(0)})^{1/2} e^{-\beta E_K^{(0)}} , \quad \beta E_K^{(0)} \gg 1 . \quad (3.16)$$

By comparing this result with the zero-winding-number result¹ ($\lambda = 0$), we see that

$$\langle n_{\text{tot}} \rangle = \langle n_0 \rangle \cosh\beta\lambda , \quad (3.17)$$

where $\langle n_0 \rangle$ is the total density of kinks and antikinks when $\lambda = 0$:

$$\langle n_0 \rangle \cong \left(\frac{2}{\pi} \right)^{1/2} \frac{2}{d} (\beta E_K^{(0)})^{1/2} e^{-\beta E_K^{(0)}} . \quad (3.18)$$

The average winding-number density is given by

$$\langle n_w \rangle = - \frac{\partial}{\partial \lambda} \Omega(T, L, \lambda) , \quad (3.19)$$

where Ω is the thermodynamic potential

$$\Omega(T, L, \lambda) = -k_B T \ln \Xi(T, L, \mu = 0, \lambda) . \quad (3.20)$$

Thus,

$$\begin{aligned} \langle n_w \rangle &= k_B T \frac{\partial z}{\partial \lambda} \\ &= \langle n_0 \rangle \sinh\beta\lambda , \end{aligned} \quad (3.21)$$

$$= \langle n_{\text{tot}} \rangle \tanh\beta\lambda . \quad (3.22)$$

This last equation makes apparent the close analogy with the average magnetization ($\langle n_w \rangle$) as a function of a magnetic field (λ) in a spin- $\frac{1}{2}$ paramagnet.¹⁵

In situations where λ is not fixed externally but rather n_w itself, we must impose the condition

$$\langle n_w \rangle = n_w , \quad (3.23)$$

which determines the winding-number potential via Eq. (3.21)

$$\lambda = k_B T \sinh^{-1}(n_w / \langle n_0 \rangle) . \quad (3.24)$$

Combining Eq. (3.22) with Eq. (3.17) then gives the average total kink density

$$\langle n_{\text{tot}} \rangle = (\langle n_w \rangle^2 + \langle n_0 \rangle^2)^{1/2} . \quad (3.25)$$

This result agrees with the speculation put forth by Currie, Fogel, and Palmer⁷ which was based on *exact* results using the transfer-operator technique.

For completeness, we present expressions for the kink and antikink densities separately. These may be obtained from Eqs. (3.2), (3.17), and (3.21):

$$\langle n_K \rangle = \frac{1}{2} (\langle n_{\text{tot}} \rangle + \langle n_w \rangle) = \frac{1}{2} \langle n_0 \rangle e^{\beta \lambda} , \quad (3.26a)$$

$$\langle n_{\bar{K}} \rangle = \frac{1}{2} (\langle n_{\text{tot}} \rangle - \langle n_w \rangle) = \frac{1}{2} \langle n_0 \rangle e^{-\beta \lambda} , \quad (3.26b)$$

where $\langle n_0 \rangle$ at low temperatures is given by Eq. (3.18)

We remark that the winding-number potential must be small enough so that $\langle n_{\text{tot}} \rangle$ is small in order for our ideal-gas phenomenology to be valid, as can

be seen from Eq. (3.17). A rough criterion is $\exp(-\beta E_K^{(0)}) \cosh \beta \lambda < < 1$ or $\beta(E_K^{(0)} - |\lambda|) > > 1$; i.e., the winding-number potential must have magnitude less than (and not too close to) the kink creation energy. Thus, the present phenomenology is not appropriate for describing incommensurate-commensurate transitions³⁻⁵ when $\lambda = E_K^{(0)}$.

IV. SUMMARY

In this paper we have extended the ideal-kink-gas phenomenology of Currie, Krumhansl, Bishop, and Trullinger¹ to include the case of nonzero winding-number density in sine-Gordon systems. By considering kinks and antikinks to be substates of a single type of "particle" and taking into account the renormalization of the kink energy due to kink-phonon phase-shift interactions, we have obtained simple expressions for the average kink and winding-number densities as a function of temperature and winding-number potential λ . Our low-temperature results

agree precisely with the exact transfer-operator results of Currie, Fogel, and Palmer.⁷

Extensions of the phenomenology developed here to (i) treat cases such as double sine-Gordon⁸ where two types of kinks (and their antikinks) are possible and (ii) develop a virial expansion in the kink density are currently being investigated.^{16,17} This latter investigation is necessary in order to extend the phenomenology to the region just above ($|\lambda| \geq E_K^{(0)}$) the commensurate-incommensurate transition⁵ (which occurs strictly at $T=0$ and is smeared by finite T); the kink-kink interactions are responsible for keeping the kink density finite⁵ when $\lambda > E_K^{(0)}$.

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- ¹J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, *Phys. Rev. B* **15**, 5567 (1980); see also the much earlier work by A. Seeger and P. Schiller, in *Physical Acoustics* edited by W. P. Mason (Academic, New York, 1966), Vol. III, p. 361, in the context of thermal kinks in dislocation lines.
- ²J. A. Krumhansl and J. R. Schrieffer, *Phys. Rev. B* **11**, 3535 (1975).
- ³See, for example, W. L. McMillan, *Phys. Rev. B* **14**, 1469 (1976); Per Bak, in *Solitons and Condensed Matter Physics*, edited by A. R. Bishop and T. Schneider (Springer-Verlag, Berlin, 1978).
- ⁴T. Ohmi and Y. Yamamoto, *Prog. Theor. Phys.* **58**, 743 (1977).
- ⁵B. Horovitz, in *Solitons and Condensed Matter Physics*, edited by A. R. Bishop and T. Schneider (Springer-Verlag, Berlin, 1978), p. 254; and (unpublished).
- ⁶N. Gupta and B. Sutherland, *Phys. Rev. A* **14**, 1790 (1976).
- ⁷J. F. Currie, M. B. Fogel, and F. L. Palmer, *Phys. Rev. A* **16**, 796 (1977).

- ⁸R. M. DeLeonardis and S. E. Trullinger (unpublished).
- ⁹L. D. Landau and E. M. Lifshitz, *Quantum Mechanics, Non-Relativistic Theory*, 2nd ed. (Pergamon, Oxford, 1965), pp. 72,73.
- ¹⁰J. Friedel, *Philos. Mag.* **43**, 153 (1952).
- ¹¹See, for example, L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968), p.353.
- ¹²J. F. Currie, *Phys. Rev. A* **16**, 1692 (1977), and references therein.
- ¹³I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products*, 4th ed. (Academic, New York, 1965), p. 317.
- ¹⁴M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, (U. S. Department of Commerce, Washington, D. C., 1970), Chap. 9.
- ¹⁵See, for example, R. K. Pathria, *Statistical Mechanics* (Pergamon, Oxford, 1972), pp.79-85.
- ¹⁶R. M. DeLeonardis and S. E. Trullinger (unpublished).
- ¹⁷R. J. McCraw and S. E. Trullinger (unpublished).