# Investigation of a class of one-dimensional nonlinear fields $*$ <sup>†</sup>

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We investigate the behavior of a class of nonlinear one-dimensional fields with symmetric and periodic interaction. The prototypical equation of this class is the sine-Gordon system. These fields have classical and static solutions with localized particlelike properties. We present a general theoretical framework to discuss the stability of these solutions under quantum and thermal fluctuations. It is shown that stability requires a phase transition of the system into an ordered equilibrium state. As an example, we calculate exactly the thermodynamics of the classical system by evaluation of a functional integral, using transfer matrix techniques. The treatment of the boundary condition, or "kink" density, as a thermodynamic variable requires a nontrivial extension of the standard methods. By a remarkable analytic continuation we show that the thermodynamic pressure is given by the eigenvalue of Hill's equation in the first unstable region. In particular, we compute the thermodynamics of the sine-Gordon field, and find that the localized behavior exhibited by the classical system at zero temperature is completely destroyed at finite temperature; i.e., the solutions are unstable with respect to thermal fluctuations.

### I. INTRODUCTION

This paper consists of an investigation of a class of nonlinear fields  $\phi(x, t)$  whose interaction is local, symmetric, and periodic in  $\phi$ . These fields satisfy a relativistically invariant field equation, given by the following (in units of the speed of light  $c = 1$ :

$$
\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} = V'(\phi) \,, \tag{1}
$$

where

$$
V'(\phi) = \frac{\partial V(\phi)}{\partial \phi} \;, \tag{2}
$$

$$
V(\phi + 2\pi) = V(\phi) \tag{3}
$$

$$
V(-\phi) = V(\phi) \tag{4}
$$

Equation (1) can be derived from the following Hamiltonian density:

$$
H(x) = \frac{1}{2}(\phi_x^2 + \pi^2) + V(\phi) , \qquad (5)
$$

where

$$
\pi(x,t) = \frac{\partial \phi(x,t)}{\partial t}, \quad \left(\phi_x \equiv \frac{\partial \phi}{\partial x}\right); \tag{6}
$$

 $\pi(x, t)$  is the conjugate field momentum. The total energy is given by an integral of the Hamiltonian density over all space (here a box of length  $L$ ),

$$
E(\pi,\phi) = \int_0^L H(x) dx.
$$
 (7)

%hen

$$
V(\phi) = 2\sin^2\frac{1}{2}\phi\,,\tag{8}
$$

Equation (1) becomes the sine-Gordon field equation. All our main results are valid for the general fields given by Eqs.  $(1)-(4)$ . For numerical and approximate analytical considerations we consider the sine-Gordon field with Eq. (8). We note that because of the periodicity property of  $V$ ,  $\phi$ is only determined modulo  $2\pi$ .

Next we discuss the classical solutions of Eqs. (1) and (8). If we impose the boundary condition on the field  $\phi(x, t)$  that

$$
\cos \phi = 1 \quad \text{at } x = \pm \infty, \quad \text{for all } t \tag{9}
$$

then the solutions of Eqs.  $(1)$  and  $(8)$  will exhibit <sup>a</sup> conserved quantity, <sup>a</sup> "kink (particle) number, " which can be defined in the following manner:

$$
N = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\partial \phi}{\partial x} dx = \frac{1}{2\pi} \left[ \phi(+\infty, t) - \phi(-\infty, t) \right],
$$
\n(10)

where  $N$  is an integer and the kink (particle) number density is given by

$$
\rho(x, t) = \frac{1}{2\pi} \frac{\partial \phi}{\partial x};
$$
\n
$$
\frac{\partial \phi}{\partial x} > 0, \text{ for kinks; } \frac{\partial \phi}{\partial x} < 0, \text{ for antikinks.}
$$
\n(11)

What we mean by the kink number  $N$  will become clearer after we discuss a kink; we will come to this point a bit later. Another constant of motion is the total energy. If  $\phi \ll 1$ , then the sine-Gordon equation reduces to the familiar Klein-Gordon (KG) equation (sin $\phi \sim \phi$ ) given by

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 $14$ 

$$
\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} = \phi \tag{12}
$$

The solutions of the KG equation are plane waves,

$$
\phi(x,t) = \phi_k e^{i(kx - \omega t)}, \qquad (13)
$$

where

 $\omega^2 = k^2 + 1$  (14)

and the energy of such a system enclosed in a onedimensional box of length  $L$  will be

$$
E/L = \omega^2 \left| \phi_{\mathbf{b}} \right|^2. \tag{15}
$$

If we look for the solutions of Eq. (1) which are of permanent profile, i.e., the velocity of propagation,  $u$ , is constant and the solutions depend upon only a single variable

$$
s = x - ut \t{,} \t(16)
$$

then Eq. (1) reduces to

$$
\frac{d^2\phi}{ds^2} = \gamma^2 V'(\phi) \,, \tag{17}
$$

where

$$
\gamma^2 = 1/(1 - u^2) \,. \tag{18}
$$

If we integrate Eq. (17) we obtain

$$
\left(\frac{d\phi}{ds}\right)^2 = \gamma^2 \left[2V(\phi) + C_1\right],\tag{19}
$$

which gives

$$
\int \frac{d\phi}{[2V(\phi) + C_1]^{1/2}} = \pm \gamma (s - s_0) ,
$$
 (20)

where  $C_1$  and  $s_0$  are constants of integration. These solutions have many interesting properties. To illustrate these properties we will specialize to such solutions of the sine-Gordon equation. In the case of the sine-Gordon equation (8), Eq. (17) looks like the equation of motion of a simple pendulum except for the sign:

$$
\frac{d^2\phi}{ds^2} = \gamma^2 \sin\phi \;, \tag{21}
$$

which has solutions of the form

$$
\phi = 4 \tan^{-1} e^{\pm \gamma (s - s_0)} \tag{22}
$$

Note the Lorentz contraction of the moving-kink (-antikink) solution through the parameter  $\gamma$ , related to the velocity of propagation,  $u$ . The two solutions (22) satisfy the boundary conditions (9) and correspond to the kink number  $\pm 1$ . The  $\pm$  signs correspond, evidently, to the two possible helicities of the solutions. These kink (antikink) solutions (22) represent localized disturbances in the field, which is the reason they are identified as particles (antiparticles). They look like

smoothed-out step functions with limiting values of  $\phi$  at  $s = \pm \infty$  differing by a factor of  $2\pi$ . We roughly define the position of a kink (antikink) by the condition

$$
\cos \phi = -1. \tag{23}
$$

Thus for the solutions (22),  $s_0$  is the position of the kink (antikink) which is moving with velocity  $u$  at time  $t$ .

We can define a profile function  $P_r(s)$  by

$$
E/L = \omega^2 |\phi_k|^2.
$$
 (24)

For solutions given by Eq. (22),  $P_r(s)$  has the form

$$
P_r(s) = \mathrm{sech}^2[\gamma(s - s_0)] \tag{25}
$$

This function is a maximum at the position of the kink (antikink) and vanishes exponentially as s  $+ \pm \infty$ .

The energy of a moving kink is

$$
E=8\gamma\,\, ,\qquad \qquad (26)
$$

and the rest energy of a kink is

$$
E=8.
$$
 (27)

We can obtain the static solution for kinks (antikinks) by putting  $\gamma = 1$  in Eq. (22):

$$
\phi_0 = 4 \tan^{-1} e^{\pm (x - x_0)} \tag{28}
$$

We can now see that the kink number  $N$  defined by Eq. (10) is nothing but

$$
N = (the number of kinks minus the number of antikinks).
$$
\n(29)

Thus conservation of kink number is similar to conservation of baryon number in particle physics. It is natural to consider, as the name implies, an antikink as an antiparticle of a kink. Furthermore, two kinks (or antikinks) are always separated by a point where the profile function vanishes; this geometrical effect may usefully be considered as a classical version of the exclusion principle.

Returning to Eq. (21), a second set of solutions is given as

$$
F(\frac{1}{2}\phi \big| - 4\gamma^2/b^2) = \frac{1}{2}b(s - s_0), \qquad (30)
$$

where

$$
\phi(s=0)=0 \text{ and } \frac{d\phi}{ds}\bigg|_{s=0}=b,
$$
\n(31)

i.e.,  $b$  is related to the average kink pressure.  $F$  is the incomplete elliptic integral of the first kind with parameter  $(-4\gamma^2/b^2)$ .

Physically these solutions correspond to a kink crystal with lattice constant  $d$ , which is given by

$$
d = 2\sqrt{m} K(m) , \qquad (32)
$$

$$
m = 4\gamma^2/(b^2 + 4\gamma^2) \tag{33}
$$

 $K(m)$  is the complete elliptic integral of the first kind with parameter m. At  $\gamma(s-s_0) = \frac{1}{2}d$ ,

The profile function  $P_r(\gamma(s - s_0))$  can be defined in the same way as Eq. (24), i.e.,

$$
P_r[\gamma(s-s_0)] = \sin^2 \frac{\phi}{2}
$$
  
=  $(1-m) \frac{\sin^2[b(s-s_0)/2(1-m)^{1/2}|m]}{\sin^2[b(s-s_0)/2(1-m)^{1/2}|m]},$ 

where

$$
\begin{aligned} \n\sin\left[\frac{b(s-s_0)}{2(1-m)^{1/2}}\right]m\,,\\ \n\sin\left[\frac{b(s-s_0)}{2(1-m)^{1/2}}\right]m\end{aligned}
$$

are the Jacobian elliptic functions with parameter m.

The energy of interaction between two kinks (antikinks) separated by a distance  $d$  is given by

$$
E = (8/\sqrt{m})[E(m) - \frac{1}{2}(1-m)K(m)], \qquad (35)
$$

where  $E(m)$  is the complete elliptic integral of the second kind with parameter  $m$ .  $E_I$  is the average energy per kink of the kink crystal when  $\gamma = 1$ . As discussed by Perring and Skyrme,<sup>1</sup> the potential between two similar particles, i.e., kink-kink (antikink-antikink), will be given by

$$
V \sim \begin{cases} 32e^{-d} & \text{as } d \to \infty, \\ V \sim \end{cases}
$$
 (36)

$$
\int 2\pi^2/d \quad \text{as } d \to 0 \,, \tag{37}
$$

where  $d$  is the distance between two kinks (antikinks) given by Eq. (32). Thus two identical particles separated by a large distance will behave like free particles. At close distances there will be a strong repulsion. The origin of this repulsion is quite clear. It comes from the nature of the boundary conditions, Eq. (9):  $\phi$  has to change by  $2\pi$ over a small distance, implying a large field gradient and a large addition to the gradient term in the Hamiltonian density given by Eq. (5).

By a similar analysis one can find that the asymptotic potential between a kink and an antikink behaves as given by Eq. (36) except for a change in sign, i.e., the force is attractive for dissimila particles. At small distances the boundary conditions match, so that  $\phi$  assumes a nearly constant value; hence there is a potential well of maximum depth equal to one kink rest mass.

Let us now look at the scattering of  $N$  kinks (antikinks) as discussed by Hirota.<sup>2</sup> Hirota has found some  $ad hoc$  exact solutions of the sine-Gordon equation. When he considers the scattering of N kinks (antikinks), he finds out that after colliding with other kinks, a kink conserves its

identity, the effect of collision being only to cause a time delay or to introduce a phase shift in the outgoing state; there is no diffraction.

Now we will briefly consider the case of small oscillations about a single kink  $Eq. (28)$  and a kink crystal solution [Eq. (30)]. Let

$$
\phi(x,t) = \phi_0(x) + \psi(x,t) , \qquad (38)
$$

where

(34)

$$
\psi(x,t) = \psi_k(x) e^{-i \omega t} \tag{39}
$$

 $\psi(x, t)$  are the small oscillations  $[\psi(x, t) \ll 1)]$  and  $\phi_0(x)$  is the single-kink solution. Then we find that the single-kink solution is stable against almost every variation  $\psi_k$ , the only exception being a rigid translation, against which  $\phi_0$  is in neutral equilibrium, because  $\omega^2 = 0$ . With respect to the scattering states  $\psi_k$ , the kink solution  $\phi_0(x)$  is completely transparent at any given energy of the incoming  $\psi_k$ . In this case  $k^2 = \omega^2 - 1$ , as given by Eq. (14).

The small oscillations about the periodic solution Eq. (30) also show unusual behavior. This crystal has only two bands for  $\psi_b$ : the valence band and the conduction band. The valence band in fact is made of correlated translations of the individual kinks; they are identified as the phonon mode of the kink crystal. The remaining conduction band corresponds to the renormalized Klein-Gordon bosons.

To make our discussions complete for the ground state of the classical kink crystal, let us compute various thermodynamic quantities. The groundstate energy is given by Eq. (35) and the specific volume is the same as the lattice spacing  $d$  with  $\gamma=1$ :

$$
U/N = E_I = (8/\sqrt{m}) [E(m) - \frac{1}{2}(1-m)K(m)] , \quad (40)
$$

$$
L/N \equiv d = 2\sqrt{m} K(m) , \qquad (41)
$$

$$
m = 4/(b^2 + 4), \quad \gamma = 1.
$$
 (42)

The thermodynamic pressure  $P_k$  of this system can be obtained by using the second law of thermodynamics:

$$
P_k = -\left(\frac{\partial U}{\partial L}\right)_{T=0} = \frac{2(1-m)}{m} \ . \tag{43}
$$

The equation of state can be obtained by eliminating the parameter  $m$  from Eq. (43) by using Eq. (32). We will call the pressure  $P<sub>b</sub>$  the kink pressure. Now, other thermodynamic quantities can be computed quite conveniently. The enthalpy is given by

$$
H \equiv (U + Pk L) = 8NE(m)/\sqrt{m} . \qquad (44)
$$

Also, the chemical potential at zero temperature is simply the enthalpy per kink, i.e.,

$$
\mu = 8E(m)/\sqrt{m} \tag{45}
$$

The isothermal compressibility is given by

$$
H_T \equiv -\frac{1}{L} \left( \frac{\partial L}{\partial P_k} \right)_T = \frac{1}{2P_k} \frac{E(m)}{K(m)} , \qquad (46)
$$

where  $K(m)$  and  $E(m)$  are the complete elliptic integrals of the first and second kinds, respectively.

#### II. KINK STABILITY

The kink solutions presented in Sec. I have the very nice property of being localized and massive. We easily verified that such solutions are stable against small oscillations, but we must also ask whether the particle solutions are stable against quantum and ther mal fluctuations. Otherwise any quantization or expansion scheme about classical equilibrium states' will have little meaning.

Here we wish to rephrase the stability question as a question of the existence of order in the equilibrium state of the system. Thus all of our questions concerning the nature or behavior of the sine-Gordon system mill then fit within the conventional theory of phase transitions.

First, me observe that our kinks and antikinks are nothing more (or less) than domain walls. Since the kink number itself is defined as the difference of the field at two points, divided by  $2\pi$ , then if we have a kink at the origin, to the lefthand side  $\phi$  passes through  $2\pi n$ , while to the righthand side  $\phi$  passes through  $2\pi(n+1)$ .

But certainly the existence of domain walls presupposes the existence of domains. Thus from this perspective it is only natural that one focuses attention first on the pure domain itself, and only later on the boundary between two such domains.

What we have called domains may also be termed nonequivalent vacua mhen we are considering the problem of quantization at zero temperature. We will now search for a quantity, or order parameter, to distinguish the infinity of nonequivalent equilibrium states.

Intuitively, we expect that within a domain,  $\phi$ must be pretty well localized about zero (modulo  $2\pi$ ), and not, say,  $\pm 2\pi$ . But how do we make this into a rigorous quantity? Usually in the theory of phase transitions me are able to define a longrange order by considering the expectation value of a product of operators  $A$  each located at widely separated points, i.e.,

$$
\langle A_0 A_x \rangle_{\overrightarrow{x \to \infty}} \begin{cases} 0, & \text{no order,} \\ \neq 0, & \text{order.} \end{cases}
$$
 (47)

But we cannot mimic this expression in our case, for we cannot determine  $\phi$  except modulo  $2\pi$ .

However, we can determine the difference be-

tween  $\phi$  at two arbitrarily close points, for we are dealing with a continuous field. Thus if we trace a path from point 0 to point  $x$ , we may determine

$$
\Delta \phi = \int_0^x dy \, \frac{\partial \phi}{\partial y} = \phi(x) - \phi(0) \,.
$$
 (48)

But we must almays remember that the integration is implied.

We then consider the expectation value of  $(\Delta \phi)^2$ ,

$$
\Delta^2 \equiv \left\langle \left( \int_0^x \phi_y \, dy \right)^2 \right\rangle. \tag{49}
$$

If  $\phi$  simply executed a random walk about  $\phi(0)$ , we would expect  $\Delta^2$  proportional to x for large x. On the other hand, if me are in a pure domain, me expect  $\Delta^2$  to be bounded by a constant. Thus if we define an order parameter  $Q<sub>1</sub><sup>4</sup>$ 

$$
Q = \lim_{x \to \infty} \left[ \frac{\Delta^2}{x} = \left\langle \left( \int_0^x \phi_y \, dy \right)^2 \right\rangle / x \right],\tag{50}
$$

we then expect

$$
Q \begin{cases} =0, & \text{ordered state,} \\ \neq 0, & \text{no order.} \end{cases}
$$
 (51)

(In view of the behavior of  $Q$ , it might more appropriately be termed a "disorder" parameter!)

We note that our original system is invariant under a discrete symmetry, namely, displacement of  $\phi$  by  $2\pi$ ,

$$
\phi \rightarrow \phi + 2\pi n \tag{52}
$$

If we are in the ordered region,  $Q=0$ , then we observe that this discrete symmetry is broken. Recall that the Goldstone theorem, as well as the Hohenberg, and Mermin-Wagner arguments, requires a continuous symmetry, and are thus not applicable.

Another way to view the problem is to consider the kink-number fluctuations mithin the equilibrium state. In fact,  $\Delta^2$  is the mean-square fluctuation of kink number within the volume  $x$ . Thus  $Q$  is the mean-square kink-number fluctuation per unit volume. If we have "real" kinks and antikinks created in pairs, then the net kink number mill be proportional to the square root of the total number of "real" particles (kinks plus antikinks), and thus Q will be proportional to the density of "real" particles (kinks plus antikinks). Or equivalently, the kink-antikink loops will be of macroscopic size.

On the other hand, if the pairs are "virtual," and remain paired within a distance  $\Lambda$ , then  $\Delta^2$  will be proportional to  $\Lambda$ , and  $Q=0$ . In this case, the kink-antikink loops are of finite size.

But the fluctuation of kink number about zero is

Property	Heisenberg ferromagnet	Sine-Gordon system
Nature of symmetry	Continuous, rotating $\vec{\sigma}$	Discrete, $\phi \rightarrow \phi + 2\pi n$
Nature of long-range order	Two-point correlation $S = \langle \vec{\sigma}_0 \vec{\sigma}_x \rangle$	Global correlations, $Q = \left\langle \left( \int_0^x \phi_y \, dy \right)^2 \right\rangle / x$
Ordered region (symmetry broken)	$S \neq 0$	$Q = 0$
Disordered region (symmetry restored)	$S=0$	$Q \neq 0$
Nature of associated excitations in ordered region	Massless Goldstone bosons	Massive domain walls, fermions

TABLE I. <sup>A</sup> comparison of the properties of the order parameter of the Heisenberg ferromagnet and the sine-Gordon system.

determined by the behavior of the chemical potential  $\mu(\rho, T)$  with vanishing kink-number density  $\rho$ . Thus if  $\mu(\rho) \rightarrow \mu_0$  as  $\rho \rightarrow 0$ , then the mean-square fluctuation of kink number  $\Delta^2$  is bounded by a constant and  $Q = 0$ . On the other hand, if  $\mu(\rho) \rightarrow \mu_1 \rho$ as  $\rho \rightarrow 0$ , then  $\Delta^2$  will be proportional to L, and  $Q\neq 0$ .

Finally, we note that the rest energy  $m_0$  of a particle is given by the change in ground-state energy per particle at zero density  $\rho$ . But this is simply the chemical potential at  $\rho$ ,  $T = 0$ . Thus

$$
m_0 = \lim_{\substack{\rho \to 0 \\ T \to 0}} \mu(\rho, T) , \qquad (53)
$$

and if  $Q = 0$  when  $T = 0$ , then the rest mass is finite.

The previous considerations appear in striking contrast to the analogous Goldstone theorem for continuous symmetries. The comparison is summarized in Table I.

#### III. PARTITION FUNCTION

Here we will evaluate the partition function for the classical nonlinear fields  $\phi(x, t)$  described by Eq. (1) with  $V(x)$  given by Eqs. (3) and (4).<sup>5</sup> We impose the boundary conditions corresponding to the presence of  $N$  kinks in our one-dimensional system. The kink number is defined by Eq. (10).

The Hamiltonian density is given by

$$
H(x,t) = \frac{1}{2} [\pi^2 + \phi_x^2] + V(\phi) , \qquad (54)
$$

which will give the total energy as a functional,

$$
E(\pi,\phi) = \int_0^L H(x,t) dx,
$$
\n(55)

where  $L$  is the length of the one-dimensional box which holds our system.

From the form of the Hamiltonian density we can see that the total energy can be written as a sum of two contributions, one due to the conjugate momenta  $\pi(x, t)$ , kinetic energy, and the other due to the configurational part, potential energy, i.e.,

$$
E(\pi,\phi) = E_{\pi} + E_{\phi},\qquad(56)
$$

where

$$
E_{\pi} = \int_0^L \frac{\pi^2}{2} \, dx \,, \tag{57}
$$

$$
E_{\phi} = \int_0^L \left( \frac{\phi_x^2}{2} + V(\phi) \right) dx \tag{58}
$$

The canonical partition function can be written as a functional integral [i.e., a sum over all functions  $\pi(x)$ ,  $\phi(x)$ ] which will be defined more carefully later:

$$
Z(\beta, L) = \int d\pi \int d\phi \, e^{-\beta \mathbf{g} \, (\pi, \phi)}, \tag{59}
$$

$$
\beta = 1/T \tag{60}
$$

 $(k = 1$  is Boltzmann's constant), which can be split into a configurational part and a conjugate momentum part,

$$
Z = Z_{\pi} Z_{\phi} , \qquad (61)
$$

where

$$
(54) \tZ_{\pi} = \int d\pi \, e^{-\beta E_{\pi}} \t{,} \t(62)
$$

$$
Z_{\phi} = \int d\phi \, e^{-\beta E_{\phi}} \,. \tag{63}
$$

The functional integral has been used quite often in physics. Feynman has used it to reformulate quantum mechanics. Our path integral is the same as Feynman's with  $t \rightarrow ix$  and  $\hbar = 1$ . We define our path integral by replacing the continuous field  $\phi(x, t)$  by a discrete set of M field variables and dividing L into M segments of length  $\Delta x$ . Ultimately we will be interested in the continuum limit  $\Delta x = 0$ ,

$$
\Delta x = L/M \tag{64}
$$

By doing this we can replace the integral in the total-energy expression (55) by a discrete sum over all segments and replace the derivative term by finite differences. This will give us

$$
E_{\pi} = \sum_{i=1}^{M} \frac{\pi_{i+1}^2}{2} \Delta x , \qquad (65)
$$

$$
E_{\phi} = \sum_{i=1}^{M} \left[ \frac{1}{2} \left( \frac{\phi_{i+1} - \phi_i}{\Delta x} \right)^2 + V(\phi_{i+1}) \right] \Delta x , \qquad (66)
$$

where

 $\pi_i = \pi(x_i, t)$ , (67)

$$
\phi_i = \phi(x_i, t) . \tag{68}
$$

Now we impose the boundary conditions

 $\phi_1 \equiv \phi(x = 0) = a$ , (69a)

$$
\phi_{M+1} \equiv \phi(x = L) = b \tag{69b}
$$

which implies

$$
\pi_1 = \pi(x = 0) = 0,
$$
\n
$$
\pi_{M+1} = \pi(x = L) = 0.
$$
\n(70a)

This makes the evaluation of 
$$
Z_{\pi}
$$
 quite trivial, as  
it becomes a product of  $(M - 1)$  Gaussian integrals:

$$
Z_{\pi} = (2\pi/\beta \Delta x)^{(M-1)/2} \,. \tag{71}
$$

The configurational partition function  $Z_{\phi}$  is not that easy to evaluate, since it contains the nearestneighbor term plus the potential energy term. We can use the transfer matrix technique to compute Z. The transfer matrix operator connects the nearest neighbors in one dimension.

We write the partition function  $Z_{\| \phi}$  in the following way:

(65) 
$$
Z_{\phi} = \int_{-\infty}^{\infty} d\phi_2 \cdots \int_{-\infty}^{\infty} d\phi_M K(\phi_1, \phi_2)
$$

$$
\times K(\phi_2, \phi_3) \cdots K(\phi_M, \phi_{M+1}),
$$

$$
+ V(\phi_{i+1}) \Delta x, \qquad (66)
$$
(72)

where  $K(\phi_i, \phi_{i+1})$  is the transfer operator given by

$$
K(\phi_i, \phi_{i+1}) = \exp\left\{-\beta \Delta x \left[\frac{1}{2} \left(\frac{\phi_{i+1} - \phi_i}{\Delta x}\right)^2 + V(\phi_{i+1})\right] \right\},\tag{73}
$$

and the transfer matrix equation is defined as

$$
\int d\phi_i K(\phi_i, \phi_{i+1}) \Phi_n(\phi_i) = e^{-\beta \Delta x \epsilon_n} \Phi_n(\phi_{i+1}), \quad (74)
$$

where the  $\Phi_n$  form a complete set.

To incorporate the boundary conditions given by Eqs. (69), we introduce Dirac  $\delta$  functions in the expression for  $Z_{\phi}$ ,

$$
Z_{\phi} = \int_{-\infty}^{\infty} d\phi_1 \int_{-\infty}^{\infty} d\phi_2 \cdots \int_{-\infty}^{\infty} d\phi_M \int_{-\infty}^{\infty} d\phi_{M+1} \delta(\phi_1 - a) \delta(\phi_{M+1} - b) K(\phi_1, \phi_2) \cdots K(\phi_M, \phi_{M+1}), \qquad (75)
$$

where the  $\delta$  functions are defined in terms of the eigenfunctions  $\Phi_n$  of the transfer operator,

$$
\delta(\phi_i - \phi_{i-1}) = \sum_n \Phi_n^* (\phi_i) \Phi_n(\phi_{i-1}), \qquad (76)
$$

so that the partition function  $Z_{\phi}$  can be written as

$$
Z_{\phi} = \sum_{n} \sum_{m} \int_{-\infty}^{\infty} d\phi_1 \cdots \int_{-\infty}^{\infty} d\phi_{M+1} \Phi_n(a) \Phi_n^*(\phi_1) \Phi_m^*(b) K(\phi_1, \phi_2) \cdots K(\phi_M, \phi_{M+1}) \Phi_n(\phi_{M+1}). \tag{77}
$$

By using Eq. (74) M times we obtain

$$
Z_{\phi} = \sum_{n} \sum_{m} \int_{-\infty}^{\infty} d\phi_1 \Phi_n(a) \Phi_n^*(\phi_1)
$$
  
 
$$
\times \Phi_n^*(b) \Phi_m(\phi_1) e^{-\beta L \epsilon_n}
$$
  

$$
= \sum_{n} e^{-\beta L \epsilon_n} \Phi_n(a) \Phi_n^*(b) .
$$
 (78)

lt is possible to find the spectral decomposition of the operator  $K$ , because  $K$  is real and can be symmetrized easily to make it Hermitian.

Before proceeding to evaluate the thermodynamic

properties of this system, let us first look at the transfer-matrix equation. We are mainly interested in the continuum limit  $\Delta x \rightarrow 0$ , and then  $K(\phi_i, \phi_{i+1})$  is very sharply peaked in  $\phi_i$  about  $\phi_{i+1}$ , due to the Gaussian in the difference  $\phi_{i+1} - \phi_i$ . Thus if we expand  $\Phi_n(\phi_i)$  about  $\phi_{i+1}$  in a Taylor expansion and integrate over  $d\phi_i$ , only even terms will contribute and we will obtain a second-order differential equation by keeping only up to the second-order term in the difference  $\phi_{i+1} - \phi_i$ . The limits of integration can be extended over all space because of the presence of the sharply peaked Gaussian term:

$$
\int d\phi_{i} \exp\left[-\beta \Delta x \left(\frac{1}{2}\left|\frac{\phi_{i+1} - \phi_{i}}{\Delta x}\right|^{2} + V(\phi_{i+1})\right)\right] \Phi_{n}(\phi_{i})
$$
\n
$$
= \int_{-\infty}^{\infty} \exp\left[-\beta \Delta x \left(\frac{1}{2}\left|\frac{\phi_{i+1} - \phi_{i}}{\Delta x}\right|^{2} + V(\phi_{i+1})\right) \right] \left[\Phi_{n}(\phi_{i+1}) + (\phi_{i} - \phi_{i+1}) \Phi_{n}'(\phi_{i+1}) + \frac{1}{2}(\phi_{i} - \phi_{i+1})^{2} \Phi_{n}''(\phi_{i+1}) + \cdots\right]
$$
\n
$$
= (2\pi \Delta x/\beta)^{1/2} \exp\left[-\beta \Delta x V(\phi_{i+1})\right] \left[\Phi_{n}(\phi_{i+1}) + (\Delta x/2\beta) \Phi_{n}''(\phi_{i+1})\right]
$$
\n
$$
= \left(\frac{2\pi \Delta x}{\beta}\right)^{1/2} \exp\left[-\beta \Delta x V(\phi_{i+1})\right] \left(1 + \frac{\Delta x}{2\beta} \frac{d^{2}}{d\phi_{i+1}^{2}}\right) \Phi_{n}(\phi_{i+1})
$$
\n
$$
= \exp\left\{-\beta \Delta x \left[-\frac{1}{2\beta^{2}} \frac{d^{2}}{d\phi_{i+1}^{2}} - \frac{1}{2\beta \Delta x} \ln\left(\frac{2\pi \Delta x}{\beta}\right) + V(\phi_{i+1})\right] \Phi_{n}(\phi_{i+1}). \tag{79}
$$

Eq. (79) combined with Eq. (77) will give

$$
\exp\left\{-\beta \Delta x \left[ -\frac{1}{2\beta^2} \frac{d^2}{d\phi^2} - \frac{1}{2\beta \Delta x} \ln \left( \frac{2\pi \Delta x}{\beta} \right) + V(\phi) \right] \right\} \Phi_n(\phi) = e^{-\beta \Delta x \epsilon_n} \Phi_n(\phi) , \tag{80}
$$

which can be equivalently written

$$
\left[ -\frac{1}{2\beta^2} \frac{d^2}{d\phi^2} - \frac{1}{2\beta \Delta x} \ln \left( \frac{2\pi \Delta x}{\beta} \right) + V(\phi) - \epsilon_n \right] \Phi_n(\phi) = 0,
$$
\n(81)

which is a one-particle Schrödinger equation. Since  $V(\phi)$  is periodic in  $\phi$  with period  $2\pi$ , the above equation is the familiar Hill equation of the band theory of solids. To make our notations match the conventional ones we make the following transformation:

$$
q=4\beta^2\,,\tag{82}
$$

$$
a_n = 8\beta^2 \left[ \left( \epsilon_n - 1 \right) + \left( 1/2\beta \Delta x \right) \ln(2\pi \Delta x/\beta) \right], \tag{83}
$$

01

$$
a_n = 2q(\epsilon_n - 1) + (4\beta/\Delta x) \ln(2\pi \Delta x/\beta) . \tag{84}
$$

We can then rewrite Eq. (81) as

$$
\frac{d^2}{d\phi^2} + \frac{a_n + 2q[1 - V(\phi)]}{4} \Phi_n(\phi) = 0.
$$
 (85)

If we make a change of variable,

$$
v = \frac{1}{2}\pi - \frac{1}{2}\phi \tag{86}
$$

and use

$$
V(\phi) = 2\sin^2\frac{1}{2}\phi\,,\tag{87}
$$

we will then obtain Mathieu's equation

$$
\frac{d^2}{dv^2} + (a_n - 2q\cos 2v) \Phi_n(V) = 0.
$$
 (88)

It is interesting to note the relationship of  $\epsilon_n$  and the eigenvalue  $\frac{1}{4}a_n$  of Hill's equation. Let us use this relationship in rewriting the partition function  $Z_{\phi}$ :

$$
Z_{\phi} = \left(\frac{2\pi\Delta x}{\beta}\right)^{M/2} \sum_{n} \exp\left[-\beta L \left(\frac{a_n}{2q} + 1\right) \Phi_n(a) \Phi_n^*(b)\right].
$$
\n(89)

To further simplify the above expression, we must look at some properties of Hill's equation. The solutions of this equation are given by the wellknown Floquet theorem or the Bloch's theorem,

$$
\Phi_n(2\pi n + \phi) = e^{ik_n 2\pi n} \Phi_n(\phi) . \qquad (90)
$$

The energy eigenvalues  $\frac{1}{4}a_n$  of Hill's equation lie in bands as functions of the wave number  $k_n$ .

If we denote the band index by  $l$  (where  $l$  $= 0, 1, 2, \ldots$ , then for corresponding points in the different bands we note

$$
k_{n,1} = k_{n,0} + \frac{1}{2}l \tag{91}
$$

This is a very useful property in simplifying for  $Z_{\phi}$ .

To insure the presence of  $N$  kinks, we can write in Eq. (69)

$$
a=0;\quad b=2\pi N\,.
$$

Now we use Eqs. (90) and (92) to rewrite the partition function  $Z_{\phi}$ 

$$
Z_{\phi} = \left(\frac{2\pi\Delta x}{\beta}\right)^{M/2} \sum_{n} \exp\left[-\beta L \left(\frac{a_n}{2q} + 1\right) - 2\pi i N k_n\right]
$$

$$
\times |\Phi_n(0)|^2. \tag{93}
$$

The wave function  $\Phi_n(0)$  is expected to be a slowly varying function of  $k_n$ ; thus in the thermodynamic limit it will not contribute. Because of the introduction of a phase factor in  $Z_{\phi}$  one cannot immediately take the thermodynamic limit. If we use the property of the wave number  $k_n$  given by Eq. (91) we can write

$$
e^{2\pi i k_n, l^N} = (-1)^{N} e^{2\pi i k_n, 0^N}.
$$
 (94)

This clearly shows that in the thermodynamic limit we need to keep the contribution only from<br>the first band, since  $e^{-\beta L a_{n,0}/2q}$  is going to be the first band, since  $e^{-\beta L a_n}$ ,  $\frac{1}{2}a$  is going to be much larger than  $e^{-\beta L a_n}$ ,  $l^{2q}$  ( $l\neq 0$ ) in the limit

 $L \rightarrow \infty$ . Hence we can write an integral expression for  $Z_{\phi}$  over the first band only,

$$
Z_{\phi} = \left(\frac{2\pi\Delta x}{\beta}\right)^{M/2} \frac{1}{2\pi}
$$
  
 
$$
\times \int_{-1/2}^{1/2} dk \exp\left[-\beta L\left(\frac{a_0(k)}{2q} + 1\right) - 2\pi i Nk\right]
$$
  
 
$$
\times |\Phi_k(0)|^2.
$$
 (95)

Now the total partition function  $Z$  will be given by (large M)

$$
Z = \left(\frac{2\pi}{\beta}\right)^M
$$
  
 
$$
\times \int_{-1/2}^{1/2} dk \exp\left[-\beta L \left(\frac{a_0(k)}{2q} + 1\right) - 2\pi i Nk\right]
$$
  
 
$$
\times |\Phi_k(0)|^2.
$$
 (96)

It is very difficult to pick out the most significant contribution to the integral of Eq. (96), for it is determined by cancellation of phase, and not simply by picking the term with the largest magnitude. However, we may avoid this problem in a very neat manner by considering the grand canonical ensemble:

$$
\Xi(\mu,\beta,L) = \sum_{N=-\infty}^{\infty} e^{N\mu} Z_N
$$

$$
= \left(\frac{2\pi}{\beta}\right)^M \int_{-1/2}^{1/2} dk \, |\Phi_k(0)|^2
$$

$$
\times e^{-\beta L} \left(\frac{a_0(k)}{2q} + 1\right)
$$

$$
\times \sum_{N=-\infty}^{\infty} e^{-N(2\pi i k - \mu \beta)} \cdot (97)
$$

Also, from standard thermodynamic relations,  

$$
\Xi(\mu, \beta, L) = e^{PL\beta},
$$
 (98)

where  $P$  is the thermodynamic pressure. Note that in Eq. (97) the sum over N runs from  $-\infty$  to  $\infty$ . This is because we have defined the kink number  $N$  in such a way that it can take negative as well as positive values.

Now suppose that we allow the chemical potential to take imaginary values,

$$
\mu \beta = 2\pi i \lambda \tag{99}
$$

We can then immediately perform the sum over  $N$ ,

$$
\sum_{N=-\infty}^{\infty} e^{-2\pi i N (k-\lambda)} = \delta(k-\lambda).
$$
 (100)

Thus the integral of Eq. (97) is immediately performed,

$$
\Xi(\mu,\beta,L) = \left(\frac{2\pi}{\beta}\right)^M \exp\left[-\beta L \left(\frac{a_0(\lambda)}{2q} + 1\right)\right] |\Phi_{\lambda}(0)|^2.
$$
\n(101)

Taking the thermodynamic limit we obtain

$$
P\beta = \frac{M}{L} \ln \left( \frac{2\pi}{\beta} \right) - \beta \left( \frac{a_0(\lambda)}{2q} + 1 \right) .
$$
 (102)

The question of whether we may analytically continue the chemical potential back onto the real axis, and thus to physical values, is answered by investigating in detail the analytical properties of  $a_0(\lambda)$ . Fortunately, this has been done by Kohn<sup>6</sup> in connection with the band problem; the answer is affirmative. If we continue the wave vector  $\lambda$ to imaginary values  $-i\mu\beta/2\pi$ , then the first allowed band energy  $a_0(\lambda)$  becomes the energy of the first forbidden band  $-A_0(\mu \beta / 2\pi)$ . We have now arrived at the final expression

$$
\beta P(\mu,\beta) = \frac{M}{L} \ln \left( \frac{2\pi}{\beta} \right) + \frac{\beta A_0}{2q} - \beta.
$$
 (103)

There are several apparent difficulties with this expression: (i) there are too many modes, so that we cannot take the continuum limit  $(\Delta x - 0)$ ; and (ii) at low temperature the third law of thermodynamics is not satisfied (the entropy  $s \rightarrow -\infty$  instead of zero}.

The origin and resolution of these difficulties are of course well understood; we should be using quantum mechanics. They are expected whenever we treat a continuum field classically. We will avoid the first difficulty, the so-called ultraviolet catastrophe, by normalizing to the harmonic field,  $V=0$ . The thermodynamic quantities for the normalized system are then always well behaved in the continuum limit. It should, however, be kept in mind that this infinity of the higher modes may act as a thermal reservoir, allowing, for instance, the normalized specific heat to become negative by a finite amount.

We will write the pressure as a sum of two terms:

$$
P = P_0 + P' \tag{104}
$$

where

$$
P_0 = (M/L\beta) \ln(2\pi/\beta) , \qquad (105)
$$

which is the  $V=0$  limit. This is the pressure of a classical harmonic oscillator with M degrees of freedom. The corresponding average energy per mode is  $T$  and the specific heat per mode is unity (we have chosen units such that Boltzmann's constant  $k = 1$ ).

 $P'$  is the normalized pressure. We shall further divide  $P'$  into a "vacuum" part (kink number  $N = 0$ )  $P_1$  and a "kink" part  $P_2$  by

$$
P' = P_1 + P_2. \tag{106}
$$

This division has been motivated by the localized "particle" properties of kinks at  $T = 0$ . Also, it

is experimentally possible to vary  $P_1$  and  $P_2$  separately.

As explained we call the state which has no kink number present, i.e.,  $N=0$ , or equivalently, the chemical potential  $\mu = 0$ , the vacuum state:

$$
P_1(\beta) = P(\mu = 0, \beta) - P_0(\beta)
$$
  
=  $A_0(\beta)/2q - 1$ ,  
 $P_2(\mu, \beta) = P(\mu, \beta) - P(\mu = 0, \beta)$  (107)

$$
= (1/2q) [A_0(\mu \beta / 2\pi, \beta) - A_0(0, \beta)]. \quad (108)
$$

Knowing the pressures  $P_1(\beta)$  and  $P_2(\mu, \beta)$  one can derive all relevant thermodynamic functions. Next, we will consider the derivation of approximate analytic expressions for various thermodynamic functions for the sine-Gordon field. We have also performed numerical calculations of various thermodynamic quantities for the sine-Gordon field.

Let us first consider the case  $V=0$  for Eq. (85). In this case the solutions of Eq. (85) are plane waves,

$$
\Phi_n(\phi) = e^{ik_n\phi} \,, \tag{109}
$$

with

$$
a_n = 4k_n^2 - 2q = -\mu^2 \beta^2 / \pi^2 - 2q \,, \tag{110}
$$

from Eq. (99). This gives the kink pressure  $P_2$ from Eq. (108) as

$$
P_2 = \mu^2 / 8\pi^2 \,, \tag{111}
$$

which corresponds to the density of kinks

$$
\rho \equiv \left(\frac{\partial P_2}{\partial \mu}\right)_{\beta} = \frac{\mu}{4\pi^2},\qquad(112)
$$

and the equation of state is

$$
P_2 = 2\pi^2 \rho^2, \tag{113}
$$

with internal energy density

$$
u = U/N = P_2, \tag{114}
$$

which gives specific heat at constant kink density

$$
C_{\rho} = 0. \tag{115}
$$

We will expect that the results we obtain will show this behavior for the  $T \rightarrow \infty$  limit.

Now let us look at the behavior of the vacuum state, i.e.,  $\mu = 0$ , for finite q. From Eq. (107), the vacuum pressure  $P_1$  is given by

$$
P_1 = A_0(\beta)/8\beta^2 - 1.
$$
 (116)  $\mu$ 

From tables for Mathieu's equation,

$$
A_0(\beta) = 8\beta^4 - 14\beta^8 + \frac{464}{9}\beta^{12} - \cdots; \ \beta \to 0, \qquad (117)
$$

$$
A_0(\beta) = 8\beta^2 - 4\beta + \frac{1}{4} + 1/2^6 \beta + 3/2^{10} \beta^2 + \cdots; \ \beta \to \infty ,
$$

$$
(118)\qquad \qquad \rho
$$

which will give

$$
P_1 = -1 + \beta^2 - \frac{7}{4} \beta^6 + \frac{58}{9} \beta^{10} - \cdots; \ \beta \to 0, \qquad (119)
$$

$$
P_1 = -\frac{1}{2\beta} + \frac{1}{2^5 \beta^2} + \frac{1}{2^9 \beta^3} + \frac{3}{2^{13} \beta^4} + \cdots; \ \beta \to \infty.
$$
\n(120)

Using the standard thermodynamic relationship between pressure and internal energy,

$$
u_1 = -\left(\frac{\partial (P_0 \beta)}{\partial \beta}\right)_{(\mu \beta)}, \qquad (121)
$$

we can obtain two limiting values of the internal energy per unit length,

$$
u_1 = 1 - 3\beta^2 + \frac{49}{4}\beta^6 - \frac{638}{9}\beta^{10} + \cdots; \ \beta \to 0, \qquad (122)
$$

$$
u_1 = 1 + \frac{1}{2^5 \beta^2} + \frac{1}{2^8 \beta^3} + \frac{9}{2^{13} \beta^4} + \cdots; \ \beta \to \infty , \ \ (123)
$$

and the specific heat per unit length will be given by

$$
c_L = 6\beta^3 \left(1 - \frac{49}{4}\beta^4 + \frac{3190}{27}\beta^8 - \cdots \right); \quad \beta \to 0 , \tag{124}
$$

$$
c_L = \frac{1}{2^4 \beta} \left( 1 + \frac{3}{2^4 \beta} + \frac{9}{2^7 \beta^2} + \cdots \right); \ \beta \to \infty . \tag{125}
$$

Proceeding to evaluate the kink pressure  $P_2$ , we again use the approximate expression for  $A_0(\mu\beta)$  $2\pi$ ) in the limits of small and large q. Let us first consider the case of small  $q$  ( $q$ <1). In such a case we can use the "nearly free electron" approximation of the band theory of solids to derive the energy of the first forbidden region of Eq. (88). By using a second-order perturbation theory we can obtain an approximation for  $A_0(\mu\beta/2\pi)$  up to order  $q^2$ . Higher-order terms are available in the tables. In this approximation (for  $\beta \rightarrow 0$ )

$$
A_0 \left( \frac{\mu \beta}{\pi} \right) = \frac{\mu^2 \beta^2}{\pi^2} + \frac{8\pi^2 \beta^4}{\pi^2 + \mu^2 \beta^2} + \cdots \qquad (126)
$$

This will give the kink pressure  $P_2$  as

$$
P_2(\mu,\beta) \simeq (\mu^2/8\pi^2) \left[1 - 8\pi^2\beta^4/(\pi^2 + \mu^2\beta^2)\right].
$$
 (127)

Note that the first term in this expression corresponds to the value for  $V=0$ . By inverting this equation, we can obtain an expression for the chemical potential,

$$
\mu \simeq 2\pi (2P_2)^{1/2} \bigl[ 1 + 4\beta^4 / (1 + 8\beta^2 P_2) \bigr] \,. \eqno{(128)}
$$

From this expression, we note another interesting result. When  $P_2 \rightarrow \infty$ ;

$$
\mu + 2\pi (2P_2)^{1/2} = \mu (V = 0) .
$$

It is very interesting that the limit of large pressure corresponds to the limit of large temperature.

From the expression for the kink pressure we can obtain the kink density

$$
\rho \simeq (\mu / 4\pi^2) \left[ 1 - 8\pi^2 \beta^4 / (\pi^2 + \mu^2 \beta^2) \right], \tag{129}
$$

and the equation of state can be obtained by eliminating  $\mu$  from Eqs. (127) and (129):

$$
P_2 \simeq 2\pi^2 \rho^2 \left\{ 1 + 8\beta^4 / \left[ 1 + (4\pi \rho \beta)^2 \right] \right\}.
$$
 (130)

This equation of state has the limiting value given by Eq. (113) in the limit of  $\beta \rightarrow 0$  and also in the limit of  $P_2$ + $\infty$ .

The internal energy per unit length is given by

$$
U/L \simeq \mu^{2}/8\pi^{2} [1 + 24\pi^{2} \beta^{4}/(\pi^{2} + \mu^{2} \beta^{2})]
$$
  

$$
\simeq 2\pi^{2} \rho^{2} \{1 + 40\beta^{4}/[1 + (4\pi \rho \beta)^{2}]\}.
$$
 (131)

Also, the internal energy per kink can be obtained by dividing Eq. (131) by  $\rho$ ,

$$
U/N \simeq \frac{1}{2} \mu \left[ 1 + 32\pi^2 \beta^4 / (\pi^2 + \mu^2 \beta^2) \right]. \tag{132}
$$

When  $q$  is large, it is not possible to find an asymptotic expansion which is valid for all values of  $q$ . Here we will discuss an approximation which is valid for most of the region of the first forbidden band of the Mathieu equation. In this region  $a$  $\epsilon - 2q + 2\sqrt{q}$ . We find<sup>7</sup> the first term of an asymptotic expansion which is valid for large  $a$  and  $q$ .

For  $a < -2q$ , we use the Liouville transformation

$$
\xi = \int_0^v \left( -a + 2q \cos 2t \right)^{1/2} dt, \ \eta = \left( -a + 2q \cos 2v \right)^{1/4} \Phi \ , \tag{133}
$$

to turn Mathieu's equation into

$$
\frac{d^2\eta}{d\xi^2} - [1 - r(\xi)]\eta = 0, \qquad (134)
$$

where

$$
r(\xi) = (4q^2 - 2qa\cos 2v + q^2\sin^2 2v) / (-a + 2q\cos 2v)^3.
$$
\n(135)

If  $-a$  is large, then  $r(\xi)$  is small in comparison with unity, and

$$
\cosh(\mu\beta) = \cosh\left[\int_0^{\pi} \left(-a + 2q\cos 2t\right)^{1/2} dt\right] + O\left(\frac{1}{\sqrt{a}}\right).
$$
\n(136)

The quantity in the brackets is related to the complete elliptic integral of second kind,  $E(m)$ , with

$$
m = 4q/(-a + 2q) , \t\t(137)
$$

and we obtain

$$
\mu \beta = 2(-a + 2q)^{1/2} E(m) \,. \tag{138}
$$

From Eqs. (103) and (104),  $-a = 2q(P' + 1)$ , where  $P'$  is the normalized total pressure. Then

$$
m = 2/(P' + 2), \qquad (139)
$$

and the chemical potential is given by

$$
\mu = 8E(m)/\sqrt{m} \ . \tag{140}
$$

Also,  $P' = P_1 + P_2$ , where the vacuum pressure  $P_1$ is linearly dependent upon temperature in this approximation. We would like to separate the kink pressure term in  $m$ . To do that we can write

$$
m = \frac{2}{P_2 + 2} \frac{1}{1 + P_1/(P_2 + 2)} \ . \tag{141}
$$

 $P_1/(P_2+2)$  < 1, and we write

$$
m = m' - m'' \t{,}
$$
 (142)

where

$$
m' = 2/(P_2 + 2) ,
$$

$$
m'' = 2P_1 / (P_2 + 2)^2.
$$
 (143b)

Note that  $m'' \ll m'$ .

Now, we can expand  $E(m' + m'')$  about m' in a Taylor series and obtain

$$
E(m'-m'')=E(m')-m''\frac{dE}{dm'}+\frac{m''^{2}}{2}+\cdots.
$$

Finally, we can write

$$
E(m' - m'') = E(m') - (m''/2m') [E(m') - K(m')],
$$
\n(145)

where  $K(m')$  is the complete elliptic integral of the first kind. In this approximation  $P_1(T) = -\frac{1}{2}T$ . Using this fact, we obtain an expression for the chemical potential up to first order in  $T$ ,

$$
\mu = \mu_0 - \mu_1 T \,, \tag{146}
$$

where

$$
\mu_0 = (8/\sqrt{m'}) E(m'), \qquad (147)
$$

$$
\mu_1 = \sqrt{m'} K(m'). \qquad (148)
$$

If we can find the next terms of the asymptotic expansion, we would be able to find higher-order terms in the expansion for  $\mu$ . This is almost impossible to do.

We note that these expressions at  $T = 0$  K match with those at the end of Sec. I, where we had derived the thermodynamics at absolute zero. We identify  $P_k$  and  $P_2$  as the same kink pressure.

We can again check whether the limit  $P_2 \rightarrow \infty$  gives us the limiting values for  $V=0$ . In this limit

$$
\mu \beta = 2(-a + 2q)^{1/2} E(m). \qquad (138) \qquad m' \rightarrow 0, \quad E(m') = K(m') = \frac{1}{2} \pi , \qquad (149)
$$

and after using this fact we can obtain the limiting values which are the same as for  $V=0$ ,

$$
\mu^2 = 8\pi^2 P_2, \tag{150}
$$

$$
2\pi \rho = (2P_2)^{1/2},\tag{151}
$$

$$
U/N = \pi (2P_2)^{1/2}, \qquad (152)
$$

(143a)

(144)

which gives the energy per unit length as 25

$$
U/L = P_2. \tag{153}
$$

# IV. DISCUSSION 15

We have obtained most of the approximate expressions we need to know about the thermodynamic behavior of our nonlinear system; we will now discuss the implications of these results.

Let us first discuss the vacuum-state thermodynamics. We have defined the vacuum state to be the state when no kink is present. For this state the pressure  $P_1$  is a function only of temperature, as shown in Pig. l. We note from our analytic expressions that the value of the "vacuum entropy" per unit length at  $T = 0$ °K is  $-\frac{1}{2}$ . This corresponds to the entropy of the normalized Klein-Gordon equation (when the contribution of the M classical harmonic oscillators, the background, is subtracted from the Klein-Gordon equation). Thus we see that at  $T = 0$  K, the small oscillations of the sine-Gordon equation are the only contributors to the entropy. (We obtain the Klein-Gordon from the sine-Gordon equation when  $\phi \ll 1$ .) The limiting value of entropy as  $T \rightarrow \infty$  is zero. Again this limit corresponds to  $V=0$  with  $N = 0$ , and the entropy for such a solution of the wave equation is zero. These limiting values of the "vacuum entropy" explain the behavior of the specific heat for the vacuum state, which is always positive and has a hump between vanishing values at  $T = 0$  and  $T = \infty$ . At this stage one should note that the limits  $P_2 \rightarrow 0$  and  $T \rightarrow 0$  do not commute. When  $P_2$  is zero at finite temperature, we only



FIG. 1. Vacuum pressure  $P_1$  as a function of temperature.



FIG. 2. Chemical potential  $\mu$  as a function of kink pressure  $P_2$  at three fixed values of temperature.



FIG. 3. Entropy per unit lenth 8/L as a function of temperature. The upper five curves correspond to five fixed values of kink pressure  $P_2$ . The curve in the lower half is due to the vacuum part.

have the vacuum contribution. At  $T = 0$  and  $P_2 \neq 0$ , we have the kink crystal. But at  $T=0$ , if we put  $P_2 = 0$ , we will not obtain the entropy corresponding to the vacuum state. Similar behavior can be seen from the  $\mu - P_2$  graph (Fig. 2).

We have mentioned that a single-kink (-antikink) solution represents a localized disturbance in the field, which is the reason it is identified as a particle (antiparticle). The periodic solution (30) then represents an array of localized disturbances. We may also see that the kinks (antikinks) are localized by looking at the energy per kink, given by Eq. (40), as we pull the crystal apart, i.e.,  $L \rightarrow \infty$  (or equivalently make the kink pressure  $P_2\rightarrow 0$ . The energy per particle goes to a fixed value, equal to 8, which is the rest mass of a single, static kink. This illustrates the localized particle behavior of kinks. At  $T = 0$  K, we consider the ground state of our kink crystal as the periodic solution given by Eq. (30) with  $\gamma = 1$ , which represents an array of kinks arranged periodically with lattice spacing  $d$  (which is the same as the specific volume), given by Eq. (32). *d* depends upon the kink pressure  $P_2$ . All the. thermodynamic quantities for this periodic array of particles can be expressed in terms of the kink pressure.

Let us look at the isotherms in the  $\mu - P_2$  plane (Fig. 2). The intercept of the  $T = 0$  isotherm with the  $P_2 = 0$  axis represents the rest mass (=8) of a single kink. The reflection of any isotherm about the  $\mu$  =0 axis gives the curve for antiparticle. As

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we proceed to any  $T-0$  isotherm, the intercept of  $\mu$  on the P<sub>2</sub> = 0 axis vanishes. The vanishing of the intercept of  $\mu$  on the  $P_2 = 0$  axis can be interpreted as the vanishing of the rest mass of a kink, which means that the kinks are no longer localized. In other words, at any  $T\neq 0$ , thermal fluctuations completely destroy the local nature of the kinks and the massive particle behavior is lost. This behavior, of course, is consistent with the discussion of Sec. II, and simply indicates the lack of order in the equilibrium state at finite temperatures.

We have looked at the individual behavior of both the kink and the vacuum parts. Now, if we look at the behavior of the kink and the vacuum parts combined, we will find that the total entropy  $\div 0$  as  $T-0$  (for  $N\neq0$ ) and also as  $T-\infty$ , and it is negative in between the two limiting values. The specific heat  $\div 0$  and  $T \div 0$  and as  $T \div \infty$  and will be positive, with a maximum in between. We have already mentioned that the pressures  $P_1$  and  $P_2$  can be varied independently. This can be done by putting a partition in the box, a movable polarizer separating the vacuum and the kink parts. (The vacuum pressure  $P_1$  depends only upon the temperature, while the kink pressure  $P<sub>2</sub>$  depends upon both the temperature and the chemical potential. ) Therefore it is possible to vary the two parts independently and consider the total effect (Fig. 3). In such a case the combined thermodynamic quantities behave more smoothly than the individual contributions.

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