

Sine-Gordon system as a Toda lattice: Thermodynamics in the classical limit

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The Bethe-ansatz (BA) equation for the classical sine-Gordon (SG) thermodynamics is shown to reduce to the one for the classical Toda lattice within two approximations; the phonon-phonon interactions are neglected (the harmonic phonon) and solitons are treated nonrelativistically. Within these approximations the solitons in the SG model correspond to the particles in the Toda lattice. Making use of an analytical solution of the BA equation for the classical Toda lattice due to Oppen, we obtain an analytical solution of the approximate SG equation. We propose also a similar approximate BA equation for the ϕ^4 model, although the ϕ^4 model does not have the BA equation for the classical thermodynamics.

I. INTRODUCTION

The Bethe-ansatz (BA) formulation for the one-dimensional sine-Gordon (SG) system gives a complete description of the thermodynamics of the system in terms of elementary modes: solitons and breathing modes (or breathers, which are bound states of phonons).^{1,2} The free energy is formally the same as that of the free-fermion gas consisting of solitons and breathers, although there are interactions between these modes. However, the "energy spectra" of these modes are determined by a set of coupled integral equations, where the effect of the interaction between the modes is expressed by the integral kernels. In general these equations are solved numerically. Recently Chen *et al.*³ analyzed, following earlier works by Fowler⁴ and by Maki,⁵ the classical limit of these equations and obtained the free energy in the form of a double series expansion in t (the temperature measured by the soliton energy) and $e^{-1/t}$. Their results agree with an earlier calculation⁶ based on the transfer-integral method. However, it seems hopeless to obtain the exact solution to these coupled integral equations in a simple analytic form.

In this paper we present an approximate treatment, which enables us to obtain an analytical solution, of these equations in the classical limit. We introduce the harmonic phonon approximation and the "nonrelativistic" approximation for solitons. The soliton-soliton and the soliton-phonon interactions are taken into account. The approximate BA equations thus obtained are shown to be equivalent to those for the Toda lattice,^{7,8} a one-dimensional lattice with the exponential interaction between neighboring particles. The SG soliton corresponds to the particle in the Toda lattice. From the known exact solution for the Toda lattice,^{8,9} we get an approximate but analytical expression for the free energy of the SG system. Comparison with the exact numerical calculation¹⁰ shows our approximation is quite good at intermediate temperatures (say $0.1 < t < 0.4$).

Our approximation not only allows analytical solution, but also applies to nonintegrable systems like the well-known ϕ^4 model. The exact BA method works only for integrable systems. For nonintegrable systems with topo-

logical solitons, solitons have been treated only within the ideal-gas approximation (i.e., the soliton-soliton interaction neglected). As an illustration we will describe how our scheme can be applied to a class of nonlinear Klein-Gordon systems,¹¹ which includes, for example, the SG and the ϕ^4 systems.

II. TODA LATTICE

In this section we shall review some of known results for the thermodynamics of the Toda lattice, which will be used in a subsequent analysis of the sine-Gordon and other systems. The Toda lattice is a one-dimensional lattice in which the interaction potential U between neighboring particles is of the exponential form⁹

$$U(r) = ae^{-br}, \quad (1)$$

where r is the interparticle distance, and a and b are positive constants. Here we have not included a linear attraction term in Eq. (1), which can be eliminated by redefinition of the pressure of the lattice.

The classical partition function $Y(T, P, N)$ of the Toda lattice with N particles under a constant pressure P at temperature T is calculated as⁹

$$Y = \left\{ \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \int_{-\infty}^{\infty} dr \exp \left[-\beta \left(\frac{p^2}{2M} + U(r) + rP \right) \right] \right\}^N \\ = \left[\frac{1}{b\hbar} \left(\frac{M}{2\pi\beta} \right)^{1/2} (\beta a)^{-\beta P/b} \Gamma \left(\frac{\beta P}{b} \right) \right]^N, \quad (2)$$

where p and M are the momentum and the mass of the particle, $\beta = T^{-1}$ (we set $k_B = 1$), and $\Gamma(z)$ is the Γ function. The chemical potential $\mu(T, P)$, or the Gibbs free energy per particle, is given by

$$\mu = -N^{-1} T \ln Y. \quad (3)$$

Recently the classical limit [$\hbar b (aM)^{-1/2} \rightarrow 0$] of the Bethe-ansatz equation for the thermodynamics of the Toda lattice has been studied.^{7,8} In this formulation the pressure P is given by

$$P = T \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{-\beta\epsilon(p)} \quad (4)$$

as a function of T and μ , where the "energy spectrum" $\epsilon(p)$ is determined by the integral equation

$$\epsilon(p) = \frac{p^2}{2M} - \mu + T \int_{-\infty}^{\infty} \frac{dp'}{2\pi\hbar} b^{-1} \ln \left[\frac{aM}{(p-p')^2} \right] e^{-\beta\epsilon(p')}. \quad (5)$$

The last term of Eq. (5) is due to the interparticle interaction (1). Oppen⁸ finds an analytical solution of this equation and shows that Eqs. (4) and (5) lead to Eqs. (2) and (3).

III. SINE-GORDON SYSTEM

In this section we shall give an approximate description of the sine-Gordon thermodynamics in the classical limit, starting with the exact Bethe-ansatz formulation. The SG system is a model of the field theory in 1+1 dimensions

defined by the Lagrangian

$$L = \frac{\hbar}{c} \int dx \left[\frac{1}{2} \left(\frac{\partial\psi}{\partial t} \right)^2 - \frac{c^2}{2} \left(\frac{\partial\psi}{\partial x} \right)^2 - \left[\frac{mc^2}{\hbar g} \right]^2 [1 - \cos(g\psi)] \right], \quad (6)$$

where ψ is the dimensionless Bose field, m is the (bare) mass of the elementary Bose particle (we shall call it phonon), and g^2 is the dimensionless coupling constant. The classical limit is achieved by $\hbar, g, m \rightarrow 0$ and $\psi \rightarrow \infty$ while $\phi = g\psi$ (the classical field), $M = 8m/g^2$ (the classical soliton mass), and $\omega_0 = mc^2/\hbar$ are kept finite.

A. Classical limit of Bethe-ansatz equations

In the classical limit a set of coupled integral equations to be solved in the BA formulation of the SG thermodynamics can be transformed into the following set of equations:^{3,12}

$$u(\alpha) = \cosh\alpha - \frac{t}{\pi} \int_{-\infty}^{\infty} d\alpha' \frac{\cosh(\alpha - \alpha')}{\sinh^2(\alpha - \alpha')} \ln[\beta\hbar\omega_0 u(\alpha')] + \frac{1}{\pi} \int_{-\infty}^{\infty} d\alpha' \operatorname{sech}(\alpha - \alpha') [g_s(\alpha') + g_{\bar{s}}(\alpha')], \quad (7)$$

$$\ln[g_s(\alpha)] - \beta\mu = \ln[g_{\bar{s}}(\alpha)] + \beta\mu$$

$$= -\frac{1}{t} \cosh\alpha + \frac{1}{\pi} \int_{-\infty}^{\infty} d\alpha' \operatorname{sech}(\alpha - \alpha') \ln[u(\alpha')] - \frac{1}{2\pi t} \int_{-\infty}^{\infty} d\alpha' \ln \left[\frac{\cosh(\alpha - \alpha') + 1}{\cosh(\alpha - \alpha') - 1} \right] [g_s(\alpha') + g_{\bar{s}}(\alpha')], \quad (8)$$

where $t = T/Mc^2$ is the reduced temperature, $\omega_0 u(\alpha)$ can be interpreted as the phonon frequency of the wave number $k = (\omega_0/c) \sinh\alpha$, and $g_s(\alpha)$ and $g_{\bar{s}}(\alpha)$ are related to the distribution functions of solitons and antisolitons in the rapidity (α) space. These equations are simple extensions of those obtained by Chen *et al.*³ and by Timonen *et al.*¹² to the case of nonvanishing chemical potential μ of the soliton (the chemical potential of the antisoliton is $-\mu$). The second and third terms of Eq. (7) represent the effects of the phonon-phonon and the phonon-soliton interactions; the second and third terms of Eq. (8) the soliton-phonon and the soliton-soliton interactions.

When the coupled integral equations (7) and (8) are solved for u , g_s and $g_{\bar{s}}$, the thermodynamic potential $\Omega(T, \mu)$ per unit length is obtained by

$$\beta c \omega_0^{-1} \Omega = \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} \cosh\alpha \ln[\beta\hbar\omega_0 u(\alpha)] - \frac{1}{t} \int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} \cosh\alpha [g_s(\alpha) + g_{\bar{s}}(\alpha)]. \quad (9)$$

The Helmholtz free energy F per unit length is related to Ω by

$$\Omega = F - \mu(n_s - n_{\bar{s}}), \quad (10)$$

where n_s and $n_{\bar{s}}$ are the densities of solitons and antisolitons. Chen *et al.*³ and Timonen *et al.*¹² solved Eqs. (7) and (8) in the case that $\mu = 0$ by iteration and obtained the free energy $F = \Omega(\mu = 0)$ in a double series in t and $e^{-1/t}$, which agrees with the earlier calculation⁶ based on the transfer-integral method. Their calculation can readily be extended to the case of nonzero chemical potential provided that $\beta(Mc^2 - |\mu|) \gg 1$. In Appendix A we give the double series for the thermodynamic potential Ω in this case.

B. Approximation

We shall now introduce important approximations to Eqs. (7)–(9), which will be reasonable at low temperatures. We first neglect the second term of Eq. (7); this corresponds to the harmonic phonon approximation. As seen by insertion of Eq. (7) into Eq. (9), the contribution from the last term of Eq. (7) to the thermodynamic potential is higher order in t than the second term of Eq. (9). So we neglect also the last term of Eq. (7). Then we simply have $u(\alpha) \simeq \cosh\alpha$, or (in a more familiar form)

$$\omega_k = (\omega_0^2 + c^2 k^2)^{1/2}, \quad (11)$$

where $\omega_k = \omega_0 \cosh \alpha$ and $k = (\omega_0/c) \sinh \alpha$. Second, we introduce the nonrelativistic, or low-energy, approximation for solitons (and antisolitons); this means that we assume

$$\ln[g_s(\alpha)] - \beta\mu = \ln[g_s(\alpha)] + \beta\mu \simeq -\frac{1}{t}(1 + \frac{1}{2}\alpha^2) + \ln 2 - \frac{1}{\pi t} \int_{-\infty}^{\infty} d\alpha' \ln \left| \frac{2}{\alpha - \alpha'} \right| [g_s(\alpha') + g_s(\alpha')], \quad (12)$$

where we have performed the integral

$$\int_{-\infty}^{\infty} d\alpha' \operatorname{sech}(\alpha - \alpha') \ln(\cosh \alpha') = \pi \ln(\cosh \alpha + 1) \simeq \pi \ln 2$$

to evaluate the soliton-phonon interaction term. It is convenient to introduce the momentum $p = Mc \sinh \alpha \simeq Mc \alpha$ of soliton and a new function $\varepsilon(p)$ defined by

$$e^{-\beta\varepsilon(p)} \equiv \beta \hbar \omega_0 [g_s(\alpha) + g_s(\alpha)]. \quad (13)$$

Equation (12) is now rewritten as

$$\varepsilon(p) = \frac{p^2}{2M} - \tilde{\mu} + T \int_{-\infty}^{\infty} \frac{dp'}{2\pi \hbar} \frac{2c}{\omega_0} \ln \left| \frac{2Mc}{p - p'} \right| e^{-\beta\varepsilon(p')}, \quad (14)$$

where the “effective chemical potential” $\tilde{\mu}$ is given by

$$\tilde{\mu} = T \ln[2 \cosh(\beta\mu)] + T \ln(2\beta \hbar \omega_0) - Mc^2. \quad (15)$$

After these approximations the formula for the thermodynamic potential, Eq. (9), becomes

$$\Omega - F_{\text{ph}} \simeq -T \int_{-\infty}^{\infty} \frac{dp}{2\pi \hbar} e^{-\beta\varepsilon(p)}, \quad (16)$$

where

$$F_{\text{ph}} = T \int_{-\infty}^{\infty} \frac{dk}{2\pi} \ln(\beta \hbar \omega_k) \quad (17)$$

is the free-energy density of the (classical) harmonic phonon. A set of equations (14) and (16) describes approximately the thermodynamics of the classical SG system at low temperatures.

We note that Eqs. (14) and (16) are equivalent to Eqs. (5) and (4), the BA equations for the Toda lattice. The correspondence between parameters in the Toda and the SG systems are listed in Table I. Obviously the Toda particle corresponds to the SG soliton. From this correspondence and the exact result for the Toda lattice, Eq. (3)

TABLE I. Correspondence between parameters in the Toda and the sine-Gordon systems.

Toda	Sine-Gordon
a	$4Mc^2$
b	ω_0/c
P	$F_{\text{ph}} - \Omega$
μ	$\tilde{\mu}$

the rapidity α of the soliton is small compared to unity (note that the rapidity of the phonon can take on large values even at low temperatures). We thus approximate Eq. (8) as

with Eq. (2), we can readily write down the result for the SG system:

$$2 \cosh(\beta\mu) \left(\frac{2}{\pi t} \right)^{1/2} e^{-1/t} \left(\frac{t}{4} \right)^z \Gamma(z) = 1, \quad (18)$$

where

$$z = \beta c \omega_0^{-1} (F_{\text{ph}} - \Omega). \quad (19)$$

Equation (18), which is the central result of this paper, determines the thermodynamic potential Ω as a function of the temperature T and the chemical potential μ .

In some limiting cases asymptotic solutions of Eq. (18) can be obtained. If $\beta(Mc^2 - |\mu|) \gg 1$, for example, z is exponentially small and we can use the formula

$$\ln \Gamma(z) = -\ln z - z \ln \gamma + \sum_{n=2}^{\infty} (-1)^n n^{-1} \zeta(n) z^n, \quad (20)$$

where $\gamma = 1.781 \dots$ is the Euler constant and $\zeta(n)$ the Riemann ζ function. Substitution of Eq. (20) into Eq. (18) yields

$$\beta c \omega_0^{-1} (F_{\text{ph}} - \Omega) = \rho_0 - B_2 \rho_0^2 + B_3 \rho_0^3 - B_4 \rho_0^4 + \dots, \quad (21)$$

where

$$\rho_0 = 2 \cosh(\beta\mu) \left(\frac{2}{\pi t} \right)^{1/2} e^{-1/t} \quad (22)$$

is the total density of solitons and antisolitons multiplied by c/ω_0 in the ideal-gas approximation,¹³ and the “virial coefficients” B_n are given by

$$B_2 = \ln(4\gamma/t), \quad (23a)$$

$$B_3 = \frac{3}{2} B_2^2 + \frac{1}{2} \zeta(2), \quad (23b)$$

$$B_4 = \frac{8}{3} B_2^3 + 2B_2 \zeta(2) + \frac{1}{3} \zeta(3), \quad (23c)$$

$$B_5 = \frac{125}{24} B_2^4 + \frac{25}{4} B_2^2 \zeta(2)$$

$$+ \frac{5}{3} B_2 \zeta(3) + \frac{5}{8} \zeta^2(2) + \frac{1}{4} \zeta(4). \quad (23d)$$

Comparing Eq. (21) with the double-series result (A5) obtained by solving the complete Bethe-ansatz equations (7)–(9) iteratively, we find that our formula (18) correctly gives leading order terms in t . Asymptotic expansions of Eq. (18) in other limiting cases are given in Appendix B and compared with earlier works^{14,15} based on the transfer-integral method.

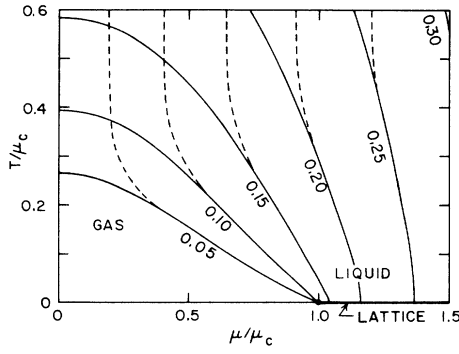


FIG. 1. Soliton density contours of the sine-Gordon system in the μ - T plane. The solid (dashed) lines indicate $n = n_s + n_{\bar{s}}$ ($w = n_s - n_{\bar{s}}$), where n_s and $n_{\bar{s}}$ are the densities of solitons and antisolitons. The numbers attached to the lines are the values of n and w multiplied by c/ω_0 .

C. Soliton density and specific heat

Once Eq. (18) is solved for z , the total number density n of solitons and antisolitons is calculated by

$$n = n_s + n_{\bar{s}} = - \left[\frac{\partial \Omega}{\partial \bar{\mu}} \right]_T = \frac{\omega_0}{c} \left[\ln \left[\frac{4}{t} \right] - \psi(z) \right]^{-1}, \quad (24)$$

where $\psi(z)$ is the digamma function. The difference of n_s and $n_{\bar{s}}$, or the “winding number density” w , is given by

$$w = n_s - n_{\bar{s}} = - \left[\frac{\partial \Omega}{\partial \mu} \right]_T = n \tanh(\beta \mu). \quad (25)$$

To derive the second equalities in Eqs. (24) and (25), we have evaluated n_s and $n_{\bar{s}}$ separately by introducing two chemical potentials μ_s and $\mu_{\bar{s}}$ of solitons and antisolitons and set $\mu_s = -\mu_{\bar{s}} = \mu$ afterward.¹⁶

In Fig. 1 we depict contours of equal soliton density in the μ - T plane calculated from Eqs. (18), (24), and (25). The solid (dashed) lines indicate contours of n (w). On the line $\mu = 0$ we have $w = 0$; w is antisymmetric with respect to μ , while n is symmetric. At lower left part of Fig. 1 the soliton density is exponentially small and the system can be regarded as being in a “soliton-gas phase.” The expansion (21) is valid in this region and hence Eq. (24) yields

$$n = (\omega_0/c)(\rho_0 - 2B_2\rho_0^2 + 3B_3\rho_0^3 - 4B_4\rho_0^4 + \dots). \quad (26)$$

On the line $T = 0$ we have a “soliton lattice,” or a “discommensuration lattice,” ($n \neq 0$) for $\mu > \mu_c = Mc^2$, while $n = 0$ for $\mu < \mu_c$. The soliton lattice melts at nonzero temperatures due to thermal fluctuations. The system may be considered as being in a “soliton-liquid phase” in the lower right region in Fig. 1, where the asymptotic behavior of the system as $T \rightarrow 0$ is qualitatively different from that in the soliton-gas phase.^{14,15} There is, however, no clear boundary between the soliton-gas and the soliton-liquid phases.

To illustrate the behavior of the system near the singu-

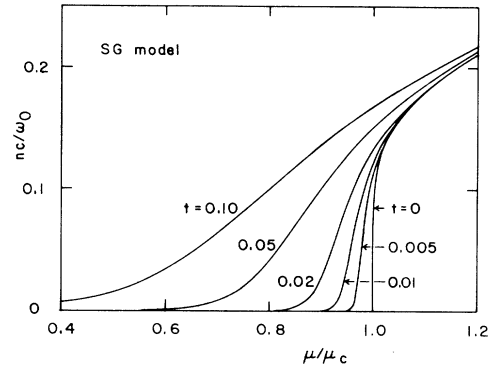


FIG. 2. The soliton density $n = n_s + n_{\bar{s}}$ of the SG system as a function of μ at low temperatures.

lar point at $T = 0$ and $\mu = \mu_c$, we calculate n at low temperatures and plot it in Fig. 2 as a function of the chemical potential μ . In the ranges of T and μ shown in Fig. 2, n is indistinguishable from w , that is $n_{\bar{s}} \simeq 0$. At $T = 0$, Eqs. (18), (24) and (25) yield $n = w$ and

$$\mu/\mu_c - 1 = 4e^{-\omega_0/cn}(1 + \omega_0/cn) \quad (27)$$

for $\mu > \mu_c$ (see Appendix B). This result agrees with the leading term of the asymptotic expansion of the exact result¹⁷ in the critical region $(\mu/\mu_c - 1) \ll 1$. Outside this region the “relativistic effect” becomes important and our approximation becomes inadequate.

The temperature dependence of the total density n of solitons and antisolitons obtained from Eq. (24) for $\mu = 0$ is shown in Fig. 3, where our result is compared with the soliton density observed in molecular-dynamics simulations.^{18–20} The data points indicate observed average number N of solitons and antisolitons, and the error bars the statistical error $\pm \sqrt{N}$. In the same figure the results of the virial expansion, Eq. (26), are also plotted with thin lines; the numbers attached them represent the orders of approximation. For example, line 1 represents the ideal-gas approximation and line 5 the fifth virial approximation.

Finally, we calculate the specific heat

$$C = -T \left[\frac{\partial^2 \Omega}{\partial T^2} \right]_{\mu}. \quad (28)$$

For simplicity we consider the case that $\mu = 0$. In this case substitution of Eq. (19) into Eq. (28) yields

$$\begin{aligned} c\omega_0^{-1}(C - C_{\text{ph}}) = \beta^2 \frac{\partial^2 z}{\partial \beta^2} &= \left[\frac{1}{t} + z - \frac{1}{2} \right]^2 \psi'(z) \left[\frac{nc}{\omega_0} \right]^3 \\ &+ \left[\frac{2}{t} + 2z - 1 \right] \left[\frac{nc}{\omega_0} \right]^2 \\ &+ \left[z - \frac{1}{2} \right] \frac{nc}{\omega_0}, \end{aligned} \quad (29)$$

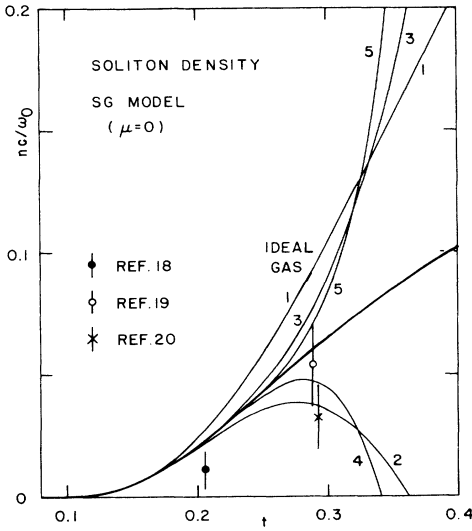


FIG. 3. Temperature dependence of the soliton density $n = n_s + n_x$ of the SG system for $\mu=0$. The thick line is calculated from Eq. (24). Thin lines are the virial expansion results [Eq. (26)]: For example, line 1 indicates the ideal-gas approximation and line 5 the fifth-order virial approximation. The data points are taken from the molecular-dynamics simulations (Refs. 18–20).

where C_{ph} is the specific heat of the harmonic phonon gas and $\psi'(z)$ is the trigamma function. We have used Eqs. (18) and (24) to derive the second equality in Eq. (29). This result is shown in Fig. 4 and compared with the exact numerical calculation¹⁰ based on the transfer-integral method. The agreement seems quite good. The discrepancy at low temperatures (say $t < 0.1$) mainly comes from the anharmonicity of the phonon, and that at somewhat higher temperatures is due to both the anharmonicity and the relativistic effect. The result of the ideal-gas approximation¹¹

$$c\omega_0^{-1}(C - C_{\text{ph}}) = 2 \left[\frac{2}{\pi t} \right]^{1/2} \left[\frac{1}{t^2} - \frac{1}{t} - \frac{1}{4} \right] e^{-1/t} \quad (30)$$

is also shown in Fig. 4, which fails to describe the peak around $t \simeq 0.22$ both in its height and position. Therefore the present solution makes a great improvement over the ideal-gas approximation.

IV. NONLINEAR KLEIN-GORDON SYSTEMS

The approximate Bethe-ansatz equation (14) for the sine-Gordon system is simple enough to easily write down similar equations for other systems. As an illustration we consider a class of nonlinear Klein-Gordon (KG) systems,¹¹ which includes, for example, the SG and the ϕ^4 systems. The BA method works only for the SG model among these systems. Fortunately, however, we have a recipe (the ideal-gas phenomenology^{11,21}) how to describe the thermodynamics of these systems in terms of solitons

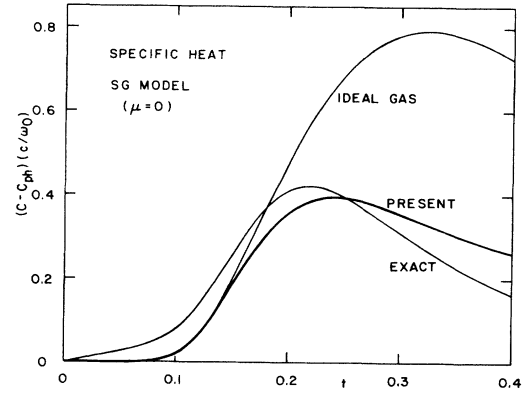


FIG. 4. Temperature dependence of the specific heat C of the SG system for $\mu=0$. The harmonic phonon contribution C_{ph} is subtracted. The thick and the thin lines are calculated from Eq. (29) and (30), respectively, which are compared with the exact calculation of Schneider and Stoll (Ref. 10).

and phonons within the ideal-soliton-gas approximation (and the harmonic phonon approximation²²). According to this theory Eq. (14) can be viewed as a simple extension of the ideal-gas phenomenology to a nonideal soliton gas, or a “soliton fluid.”

The nonlinear KG system we consider is defined by the Lagrangian (6) with $1 - \cos(g\psi)$ replaced by a dimensionless potential $V(g\psi)$ which has at least two degenerate minima to support topological solitons.¹¹ We consider here two types of potentials, (singly) periodic potentials and double-well potentials. Let ϕ_1 and ϕ_2 ($\phi_1 < \phi_2$) be locations of adjacent minima of the potential $V(\phi)$. We assume that $V(\phi)$ is symmetric about the midpoint ϕ_m of the potential barrier lying between ϕ_1 and ϕ_2 [$\phi_m = \frac{1}{2}(\phi_1 + \phi_2)$]. It is convenient to set $V(\phi_1) = 0$ and scale V so that $d^2V/d\phi^2 = 1$ at $\phi = \phi_1$; the dispersion relation of harmonic phonon is then given by Eq. (11). The SG ($V = 1 - \cos\phi$) and the ϕ^4 [$V = \frac{1}{8}(\phi^2 - 1)^2$] potentials are typical examples of periodic and double-well potentials, respectively. The classical limit is achieved in the same way we described in the SG case but the classical soliton mass M is now given by

$$M = mg^{-2} \int_{\phi_1}^{\phi_2} d\phi [2V(\phi)]^{1/2}. \quad (31)$$

According to the ideal-gas phenomenology for the nonlinear KG system,¹¹ the thermodynamic potential Ω of the system per unit length is obtained as a sum of contributions from harmonic phonons and an ideal gas of solitons. The phonon part F_{ph} is given by Eq. (17) and the soliton part Ω_s^{id} by

$$\Omega_s^{\text{id}} = -\lambda T \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{-\beta E^*(p)}. \quad (32)$$

The thermally renormalized soliton energy E^* is given by

$$E^*(p) = Mc^2 + \frac{p^2}{2M} - T \ln(2\sqrt{v\beta\hbar\omega_0}), \quad (33)$$

where ν is a model-dependent numerical constant defined by²¹

$$\nu = \frac{m}{8Mg^2} (\phi_2 - \phi_1)^2 \times \exp \left[2 \int_{\phi_m}^{\phi_2} d\phi \{ [2V(\phi)]^{-1/2} - (\phi_2 - \phi)^{-1} \} \right]. \quad (34)$$

We have $\nu=1$ and $\nu=3$ for the SG and the ϕ^4 systems. The last term of Eq. (33) (the thermal renormalization of the soliton mass) represents the change in phonon free energy due to the interaction with a soliton. The prefactor λ in Eq. (32) is given by

$$\lambda = \begin{cases} 2 \cosh(\beta\mu) & \text{for periodic potentials,} \\ 1 & \text{for double-well potentials.} \end{cases} \quad (35)$$

This factor is related with a degree of freedom which Miyashita and Maki²² called ‘‘color,’’ or topological constraint on configuration of solitons and antisolitons in the real space.¹¹ In the system with double-well potential, a soliton is always followed by an antisoliton (and vice versa), whereas there is no restriction on the sequence of solitons and antisolitons in the system with periodic potential. Because of this constraint $n_s = n_{\bar{s}}$ (therefore $\mu=0$) in the former system, while the latter system can have nonvanishing winding number as we have seen in the SG case.

If we neglect the last term (the soliton-soliton interaction) in Eq. (14), Eq. (16) reduces to the ideal-gas theory, Eq. (32), as expected. We further notice that the integral kernel in Eq. (14)

$$(2c/\omega_0) \ln(2Mc/|p-p'|) \quad (36)$$

is the spatial shift $\Delta(p,p')$ of the trajectory of a soliton of momentum p caused by a collision with a soliton of momentum p' . The corresponding quantity for the class of nonlinear KG systems is obtained as

$$\Delta(p,p') = (2c/\omega_0) \ln(2\sqrt{\nu}Mc/|p-p'|) \quad (37)$$

if we assume scatterings of solitons are elastic.²³ The constant ν in Eq. (37) is given by Eq. (34). We are thus led to

$$\varepsilon(p) = \frac{p^2}{2M} - \tilde{\mu} + T \int \frac{dp'}{2\pi\hbar} \Delta(p,p') e^{-\beta\varepsilon(p')}, \quad (38)$$

with

$$\tilde{\mu} = T \ln(2\sqrt{\nu}\lambda\beta\hbar\omega_0) - Mc^2. \quad (39)$$

We expect that a set of equations (16) and (38) approximately describes the thermodynamics of the nonlinear KG systems and can be considered as a natural extension of the ideal-gas phenomenology. The solution for the thermodynamic potential Ω is now given by

$$\lambda \left[\frac{2\nu}{\pi t} \right]^{1/2} e^{-1/t} \left[\frac{t}{4\nu} \right]^z \Gamma(z) = 1, \quad (40)$$

where z is defined by Eq. (19). This equation determines Ω as a function of t (and μ in the case of periodic potential).

Although Eq. (38) is conjectural, we believe it correctly describes the effect of the interaction between solitons as

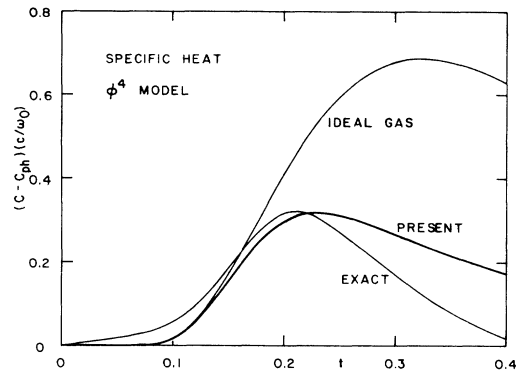


FIG. 5. Temperature dependence of the specific heat C of the ϕ^4 system ($\lambda=1$, $\nu=3$). The harmonic phonon contribution C_{ph} is subtracted. The thick and the thin lines are calculated from Eq. (29) with (42) and from Eq. (43), respectively. The exact result is taken from Ref. 10.

long as the leading order terms in t are concerned. For example, the virial expansion of Eq. (40) which is given by Eq. (21) with ρ_0 and B_2 replaced by

$$\rho_0 = \lambda \left[\frac{2\nu}{\pi t} \right]^{1/2} e^{-1/t} \quad \text{and} \quad B_2 = \ln \left[\frac{4\nu\gamma}{t} \right] \quad (41)$$

gives the correct expression for B_2 recently obtained²³ by the transfer-integral method. Figure 5 shows the specific heat of the ϕ^4 system ($\lambda=1$, $\nu=3$) calculated from Eq. (40) which is compared with the exact¹⁰ and the ideal-gas¹¹ results. Equation (29) still holds, but now n is given by

$$n = n_s + n_{\bar{s}} = \frac{\omega_0}{c} \left[\ln \left[\frac{4\nu}{t} \right] - \psi(z) \right]^{-1}. \quad (42)$$

On the other hand, the ideal-gas phenomenology gives¹¹

$$c\omega_0^{-1}(C - C_{\text{ph}}) = \lambda \left[\frac{2\nu}{\pi t} \right]^{1/2} \left[\frac{1}{t^2} - \frac{1}{t} - \frac{1}{4} \right] e^{-1/t} \quad (43)$$

for $\mu=0$. As seen in Fig. 5, the present theory gives much better description of the specific heat than the ideal-gas theory does.

V. CONCLUDING REMARKS

We have given an approximate description of the thermodynamics of the classical sine-Gordon system and its (conjectural) extension to a class of nonlinear Klein-Gordon systems. The effect of the interaction between solitons has been taken into account as an integral kernel of a conjectured Bethe-ansatz-type equation [Eq. (38)], while the interaction among phonons and relativistic effect for solitons have been neglected. Similar BA-type equations for other soliton-bearing systems can be constructed if the linear modes in the presence of a soliton and the asymptotic behavior of soliton-soliton interaction are obtained; we need these to obtain $\tilde{\mu}$ and $\Delta(p,p')$. Since

these equations are equivalent to the Toda lattice equation, the solutions like Eq. (40) can be readily obtained.

In recent neutron scattering experiments on one-dimensional magnetic systems CsNiF₃ (Ref. 24) and (CH₃)₄NMnCl₃ (TMMC) (Ref. 25) it has been reported that the observed intensity of the soliton peak is considerably smaller than what the ideal-gas theory of the SG model predicts. Since the intensity is proportional to the soliton density n , their observations are consistent with our calculation (Fig. 3); the temperature range used in these experiments is roughly $0.2 < t < 0.4$.

Although we have limited ourselves to the classical case, it is straightforward to extend Eq. (14) or (38) to the quantum case in the weak coupling limit ($g^2/8\pi \ll 1$), where the Bose statistics is applied for phonons and the second term in Eq. (15), the thermal renormalization of the soliton mass, will be modified. This version of our theory may be viewed as an extension of the Maki-Takayama theory²⁶ of quantum statistical mechanics for soliton-bearing systems within the ideal-soliton-gas approximation. In this context it is interesting to apply our scheme to a model (beyond the SG approximation) for one-dimensional easy-plane ferromagnets CsNiF₃ and (C₆H₁₁NH₃)CuBr₃ (CHAB). Recently Mikeska and Frahm²⁷ and Fogedby *et al.*²⁸ have studied the quantum effect on the specific heat of this model within the ideal-soliton-gas approximation. However, the agreement between their theories and experiments^{29,30} is still unsatisfactory; the theories give too large value of specific heat. The inclusion of the soliton-soliton interaction will considerably reduce the peak of the specific heat, as we have seen in Figs. 4 and 5, and the agreement between theory and experiment will be much improved.

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APPENDIX A: ITERATIVE SOLUTION OF EQS. (7)–(9)

We know the iterative solution of Eqs. (7)–(9) in the case that $\mu=0$, where the free energy $F=\Omega(\mu=0)$ is obtained as a double series in t and $e^{-1/t}$:^{3,5,12}

$$F = F_0 + F_1 + F_2 + F_3 + O(e^{-4/t}), \quad (\text{A1})$$

with

$$F_0 = F_{\text{ph}} - \frac{\omega_0}{c} T \left[\frac{t}{4} + \frac{t^2}{8} + \frac{3}{16} t^3 + \frac{53}{128} t^4 + \frac{297}{256} t^5 + O(t^6) \right], \quad (\text{A2a})$$

$$F_1 = -\frac{\omega_0}{c} T 2 \left[\frac{2}{\pi t} \right]^{1/2} e^{-1/t} \left[1 - \frac{7}{8} t - \frac{59}{128} t^2 - \frac{897}{1024} t^3 - \frac{75005}{32768} t^4 + O(t^5) \right], \quad (\text{A2b})$$

$$F_2 = \frac{\omega_0}{c} T \left[2 \left[\frac{2}{\pi t} \right]^{1/2} e^{-1/t} \right]^2 \times \left[\ln \frac{4\gamma}{t} - \frac{5}{4} t \left[\ln \frac{4\gamma}{t} + 1 \right] - \frac{1}{32} t^2 \left[13 \ln \frac{4\gamma}{t} + 2 \right] + O(t^3) \right], \quad (\text{A2c})$$

$$F_3 = -\frac{\omega_0}{c} T \left[2 \left[\frac{2}{\pi t} \right]^{1/2} e^{-1/t} \right]^3 \times \left[\frac{3}{2} \left[\ln \frac{4\gamma}{t} \right]^2 + \frac{\pi^2}{12} + O(t) \right], \quad (\text{A2d})$$

where F_{ph} is the free energy of the harmonic phonon given by Eq. (17). To obtain the similar result for $\mu \neq 0$, let us look at the first few steps of the iteration. The first step is to solve Eq. (7) without the last term. We shall denote the solution by $u_0(\alpha)$, which yield F_0 . The next step is to calculate the right-hand side of Eq. (8) with u replaced by u_0 and without the last term, which gives the lowest-order approximation for g_s and $g_{\bar{s}}$. It is convenient to introduce a new function $g(\alpha; \mu)$ defined by

$$g(\alpha; \mu) = \frac{1}{2} [g_s(\alpha) + g_{\bar{s}}(\alpha)]. \quad (\text{A3})$$

Note that $g = g_s = g_{\bar{s}}$ if $\mu = 0$. It is easy to find

$$g_0(\alpha; \mu) = \cosh(\beta\mu) g_0(\alpha; 0), \quad (\text{A4})$$

where g_0 is the lowest-order approximation for g . Now we substitute g_0 into the right-hand side of Eq. (7) to obtain u_1 the first-order correction to u . Both g_0 and u_1 (which is linear order in g_0) contribute to Ω_1 , the first order correction to Ω . Further iteration yields higher-order corrections. All the higher-order terms are expressed in terms of u_0 and g_0 . The n th-order terms in g_0 yield F_n in the case that $\mu = 0$. Thanks to the relation (A4) we get

$$\Omega = \Omega_0 + \Omega_1 + \Omega_2 + \Omega_3 + \cdots, \quad (\text{A5})$$

where

$$\Omega_n = \cosh^n(\beta\mu) F_n, \quad (\text{A6})$$

with F_n given by Eqs. (A2). The expansion (A5) is valid when $e^{-1/t} \cosh(\beta\mu) \ll 1$ or $\beta(Mc^2 - |\mu|) \gg 1$.

APPENDIX B: ASYMPTOTIC EXPANSIONS

We shall give asymptotic solutions of Eq. (40) [which includes the sine-Gordon case, Eq. (18), as a special case ($\nu=1$)] in some limiting cases.

A. Soliton gas: $\beta(\mu_c - |\mu|) \gg 1$

This limit is described in the text [see Eqs. (21)–(23), (26), and (41)].

B. Soliton lattice (liquid): $\mu > \mu_c$ and $t \ll 1$

When $\mu > \mu_c = Mc^2$, the quantity z diverges as $t \rightarrow 0$ like $z \sim t^{-1}$. The density of antisoliton $n_{\bar{s}}$ is much smaller than the soliton density n_s in this region; we neglect the antisolitons ($2 \cosh \beta \mu \simeq e^{\beta \mu}$). We seek the solution of the form

$$z = \frac{4v}{t} e^{-\omega_0/n_0 c} (1 + \alpha_1 t + \alpha_2 t^2 + \dots) \quad (\text{B1})$$

where n_0 will turn out to be the soliton density at $t=0$ [see Eq. (B4)]. Substituting Eq. (B1) and

$$\ln \Gamma(z) = z \ln z - z + \frac{1}{2} \ln \frac{2\pi}{z} + \frac{1}{12z} + O(z^{-3}) \quad (\text{B2})$$

into Eq. (40), we find

$$\mu/\mu_c - 1 = 4ve^{-1/\tilde{n}_0} (1 + \tilde{n}_0^{-1}), \quad (\text{B3a})$$

$$\alpha_1 = \frac{1}{8v} e^{1/\tilde{n}_0}, \quad (\text{B3b})$$

$$\alpha_2 = -\frac{1}{384v^2} \tilde{n}_0 e^{2/\tilde{n}_0}, \quad (\text{B3c})$$

where $\tilde{n}_0 = n_0 c / \omega_0$. Equation (B3a) gives \tilde{n}_0 as a function of μ . Substitution of Eq. (B1) into Eq. (42) yields the soliton density $n (=n_s$ in this limit)

$$n = n_0 \left[1 + \frac{t^2}{384v^2} \tilde{n}_0 (1 - \tilde{n}_0) e^{2/\tilde{n}_0} + O(t^3) \right]. \quad (\text{B4})$$

The thermodynamic potential Ω obtained from Eqs. (19) and (B1) agrees with that obtained by the transfer-integral method^{14,15} up to the linear order in t .

Up to the linear order in t the soliton density is independent of the temperature and Ω can be calculated based on a simple physical picture rather than abstract ‘‘Bethe-ansatz’’ or transfer-integral methods. Using the intersoliton potential²³

$$U(r) = 4vMc^2 e^{-(\omega_0/c)r}, \quad (\text{B5})$$

where r is the intersoliton distance, we obtain the dispersion relation of the soliton-lattice vibration (acoustic phonon):

$$\omega_{ac}(k) = 2n_0 v \left| \sin \frac{k}{2n_0} \right|, \quad (\text{B6})$$

$$v = 2\sqrt{v\omega_0} n_0^{-1} e^{-\omega_0/2cn_0}. \quad (\text{B7})$$

Here n_0^{-1} is the lattice constant determined by Eq. (B3a). There is also the ‘‘optical phonon’’ whose dispersion is given by Eq. (11). Therefore the thermodynamic potential Ω will be

$$\Omega = n_0 [U(n_0^{-1}) + M^* c^2 - \mu] + F_{ph} + F_{ac}. \quad (\text{B8})$$

Here we have introduced the thermally renormalized soliton mass M^* defined from Eq. (33) as

$$M^* c^2 = Mc^2 - T \ln(2\sqrt{v\beta\hbar\omega_0}). \quad (\text{B9})$$

The phonon free energies F_{ph} and F_{ac} are respectively given by Eq. (17) and

$$\begin{aligned} F_{ac} &= T \int_{-\pi n_0}^{\pi n_0} \frac{dk}{2\pi} \ln[\beta\hbar\omega_{ac}(k)] \\ &= T [n_0 \ln(2\sqrt{v\beta\hbar\omega_0}) - \omega_0/2c]. \end{aligned} \quad (\text{B10})$$

We find Eq. (B8) agrees with Eq. (B1) up to the linear order in T .

C. $\mu = \mu_c$

In this case z approaches $\frac{1}{2}$ from below as $t \rightarrow 0$. At low temperatures ($t \ll 1$) we therefore have small quantity δ defined by

$$z = \frac{1}{2} - \delta. \quad (\text{B11})$$

The logarithm of the Γ function in Eq. (40) is expanded as

$$\ln \Gamma(z) = \frac{1}{2} \ln \pi + \delta \ln(4\gamma) + \frac{\pi^2}{4} \delta^2 + \dots \quad (\text{B12})$$

Solving Eq. (40) for δ , we get

$$\delta = \frac{1}{2} \frac{\ln 2}{\ln \left[\frac{16v\gamma}{t} \right]} - \frac{\pi^2}{16} \frac{(\ln 2)^2}{\left[\ln \left[\frac{16v\gamma}{t} \right] \right]^3} + \dots \quad (\text{B13})$$

The first term of this result agrees with the transfer-integral calculation³¹ but the second term does not. Substitution of Eq. (B11) into Eq. (42) yields the soliton density n :

$$\frac{c}{\omega_0} n = \frac{1}{\ln \left[\frac{16v\gamma}{t} \right]} - \frac{\pi^2}{4} \frac{\ln 2}{\left[\ln \left[\frac{16v\gamma}{t} \right] \right]^3} + \dots \quad (\text{B14})$$

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