Second virial coefficients in soliton free energies

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The low-temperature thermodynamics of a class of one-dimensional nonlinear Klein-Gordon systems (e.g., the sine-Gordon and the ϕ^4 models) is studied by means of the transfer-integral method. A general formula for the lowest-order correction to the free energy due to the interaction between solitons is obtained. Physical interpretation of the result is given based on a simple soliton-gas picture.

I. INTRODUCTION

The statistical mechanics of topological solitons (kinks) in one-dimensional systems has attracted much attention.[1] The soliton contribution to the free energies of various systems have been studied extensively within ideal-gas approximations: Some systems (e.g., sine-Gordon and ϕ^4 models) of the nonlinear Klein-Gordon family were studied by Currie, Krumhansl, Bishop, and Trullinger[2] by means of the transfer-integral method[3] and the ideal-gas phenomenology[4] in the classical limit. The same analysis was extended to a general class of the nonlinear Klein-Gordon systems by DeLeonardis and Trullinger[5,6] and a general formula for the soliton free energy was obtained. The quantum statistical mechanics of nonlinear Klein-Gordon systems was studied by Maki and Takayama[7] in the weak-coupling limit based on the path-integral method. More recently, the Bethe-ansatz method was introduced to investigate thermodynamics of the quantum sine-Gordon system.[8,9]

The effect of soliton-soliton interactions on statistical mechanics has been considered only recently, and the study has still been restricted to the sine-Gordon system in the classical limit. The second virial correction to the free energy of a soliton gas was first obtained by the transfer-integral method[10] and then by soliton-gas phenomenology.[11] Recently, the higher-order virial terms were obtained based on the Bethe-ansatz formulation in the classical limit.[12]

The object of this paper is to derive a general formula for the second virial coefficients in the soliton free energy, in the classical limit, for a class of the nonlinear Klein-Gordon family. By using the transfer-integral method, the following formula for the soliton contribution to the free-energy density is obtained within the second virial approximation:

$$F_s = -mTC \left[\frac{2v}{\pi t} \right]^{1/2} e^{-1/t}$$

$$\times \left[1 - C \left[\frac{2v}{\pi t} \right]^{1/2} e^{-1/t} \ln \left| \frac{4v\gamma}{t} \right| \right] , \qquad (1)$$

where m is the phonon mass, T is the temperature, $t = T/M$ (M is the soliton mass), $\gamma = 1.7810 \ldots$ is the

Euler constant, and C and v are model-dependent numerical constants ($C = 2$, $v = 1$ for the sine-Gordon model; $C = 1$, $v = 3$ for the ϕ^4 model). The leading term of Eq. (1) agrees with the result of DeLeonardis and Trullinger.[5,6] The second term in the square brackets represents the lowest-order correction due to the interaction between solitons. A physical interpretation of the transfer-integral result (1) will be given. The factor C is interpreted as the "color"[13] of the solitons. The logarithmic temperature dependence of the second virial term follows from the exponential tail of the interaction between two solitons at large distances.

II. TRANSFER-INTEGRAL METHOD

The general class of nonlinear Klein-Gordon systems in one dimension is defined by the Hamiltonian[2]

$$H = \int dx \left[\frac{1}{2}\pi^2 + \frac{1}{2} \left[\frac{\partial u}{\partial x} \right]^2 + \frac{m^2}{g^2} V(gu) \right] , \qquad (2)$$

where $\pi = \partial u / \partial t$, u is the dimensionless field variable, m is a parameter with dimension of mass, and g is the dimensionless coupling constant. We use a system of units in which $\hbar = k_B = c_0 = 1$, where c_0 is the limiting velocity of the soliton. The dimensionless potential $V(\phi)$ is assumed to have at least two degenerate minima to support topological solitons.

We consider here two types of potentials, (singly) periodic potentials and double-well potentials; we exclude, for simplicity, potentials which allow more than one type of solitons, such as the double sine-Gordon potential.[14] We assume that $V(\phi) = V(-\phi)$ and it has its minimum value ($V = 0$) at $\phi = \pm\phi_0$, the period of $V(\phi)$ being $2\phi_0$ for the periodic potential. We further assume that $V(\phi)$ is scaled so that $d^2V(\phi)/d\phi^2 = 1$ at $\phi = \phi_0$; then the parameter m is the phonon mass. Familiar examples of $V(\phi)$ are the sine-Gordon ($V = 1 + \cos\phi$),[15] the ϕ^4 [$V = \frac{1}{8}(\phi^2 - 1)^2$], and the double-quadratic [$V = \frac{1}{2}(|\phi| - 1)^2$] potentials.

We define the following numerical constants constructed from the potential,[5] which will be used below:

$$\xi = \int_{-\phi_0}^{\phi_0} d\phi [2V(\phi)]^{1/2} , \qquad (3)$$

$$\eta = \int_0^{\phi_0} d\phi \{ [2V(\phi)]^{-1/2} - (\phi_0 - \phi)^{-1} \} . \qquad (4)$$

$\xi = 8$, 2/3, 1 and $\eta = \ln(4/\pi)$, ln2, 0 for the sine-Gordon, the ϕ^4, and the double-quadratic systems, respectively. We note that the soliton mass M is given by[2,5]

$$M = \xi m / g^2 . \qquad (5)$$

The classical free-energy density F is obtained exactly by using the transfer-integral method.[3] If the width of the soliton m^{-1} is large compared with the lattice constant a,[16] F can be obtained as

$$F = -Ta^{-1}\ln(aT) + (m/g)^2\epsilon_0 , \qquad (6)$$

where ϵ_0 is the lowest eigenvalue of the Schrödinger-type equation,

$$\left[-\frac{1}{2m^*}\frac{d^2}{d\phi^2} + V(\phi) \right]\psi(\phi) = \epsilon\psi(\phi) , \qquad (7)$$

with the (dimensionless) "effective mass" $m^* = (m/Tg^2)^2$. At low temperatures $t = T/M \ll 1$, ϵ_0 may be expressed as

$$\epsilon_0 = E_0 - \tau_0 , \qquad (8)$$

where $E_0 = (2m^*)^{-1/2} + O(t^2)$ [note that $(m^*)^{-1/2} = \xi t$, ξ being the constant defined by Eq. (3)] and τ_0 is an exponentially small $(\sim e^{-1/t})$ correction due to the "tunneling effect." The contribution from E_0 to F together with the first term in Eq. (6) is identical to the free energy of the classical phonon gas.[2] The tunneling contribution to the free energy, $F_s = -(m/g)^2\tau_0$, may be interpreted as the soliton free energy[2,4] (see Sec. IV).

A systematic method of evaluating τ_0 as a double-series expansion in $e^{-1/t}$ and t was given by the present author.[17] Up to the second order in $e^{-1/t}$, the "second virial coefficient," τ_0 is obtained as

$$\tau_0^{-1} = A_0 + \tau_0 A_1 \qquad (9)$$

with

$$A_0 = [\Psi'(0)]^{-1} \int_0^{\phi_M} d\phi\, G'(0,\phi)\Psi(\phi) , \qquad (10)$$

$$A_1 = -[\Psi'(0)]^{-1} \int_0^{\phi_M} d\phi\, G'(0,\phi) \int_0^{\phi_M} d\phi'\, G(\phi,\phi')\Psi(\phi') , \qquad (11)$$

where $\Psi(\phi)$ is an unnormalized "single-well wave function"[6,17]

$$\Psi(\phi) = [2V(\phi)]^{-1/4}\exp\left[\mathrm{sgn}(\phi_0 - \phi)\left(\int_{\phi_0}^{\phi} dx\,[2m^*V(x)]^{1/2} - \frac{1}{2}\int_0^{\phi} dx\,[2V(x)]^{-1/2} \right) \right][1 + O(t)] , \qquad (12)$$

and a "Green's function" $G(\phi,\phi')$ is defined by

$$G(\phi,\phi') = -2m^*\Theta(\phi'-\phi)\Psi(\phi)\Psi(\phi') \int_{\phi}^{\phi'} dx\, \Psi^{-2}(x) , \qquad (13)$$

$\Theta(\phi)$ being the step function. The functions $\Psi(\phi)$ and $G(\phi,\phi')$ are defined in the interval $0 \le \phi, \phi' \le \phi_M$, where $\phi_M = \phi_0$ $(\phi_M = \infty)$ for the periodic (double-well) potentials. In Eqs. (10) and (11), $\Psi'(\phi) = d\Psi(\phi)/d\phi$ and $G'(\phi,\phi') = \partial G(\phi,\phi')/\partial\phi$.

We note that $\Psi(\phi)$ is approximated by

$$\Psi(\phi) \simeq (\phi_0 e^{\eta})^{-1/2}\exp[-\frac{1}{2}(m^*)^{1/2}(\phi - \phi_0)^2] ,$$
$$\phi \sim \phi_0 \qquad (14)$$

in the potential well and by

$$\Psi(\phi) \simeq [2V(0)]^{-1/4}\exp\{ -\frac{1}{2}t^{-1} + [2m^*V(0)]^{1/2}\phi \} ,$$
$$\phi \sim 0 \qquad (15)$$

in the potential barrier. The constant η appearing in Eq. (14) has been defined by Eq. (4).

III. SOLITON FREE ENERGY

We shall calculate the soliton free energy, limiting ourselves to the leading order terms in t. We first note that the derivative of the Green's function can be expressed as

$$G'(0,\phi)/\Psi'(0) = (\xi t)^{-1}e^{+1/t}\Psi(\phi)\left[1 + 2(\xi t)^{-1}e^{-1/t}\int_{\phi}^{\phi_0} dx\, \Psi^{-2}(x) \right] , \qquad (16)$$

which follows from the definition of G [Eq. (13)] and the relations

$$\Psi(0)\Psi'(0) = (\xi t)^{-1}e^{-1/t} , \qquad (17)$$

$$\Psi(0)\Psi'(0) \int_0^{\phi_0} d\phi\, \Psi^{-2}(\phi) = \frac{1}{2} , \qquad (18)$$

where ξ is the constant defined by Eq. (3). Then Eqs. (10) and (11) can be rewritten as

$$A_n = 2^n(\xi t)^{-(2n+1)}e^{1/t}[C_n + 2(\xi t)^{-1}e^{-1/t}D_n] ,$$
$$n = 0,1 \qquad (19)$$

where

$$C_0 = \int_0^{\phi_M} d\phi\, \Psi^2(\phi)$$
$$= (2/C)(2\phi_0 e^{\eta})^{-1}(\pi\xi t)^{1/2} - \xi t[4V(0)]^{-1}e^{-1/t} , \qquad (20)$$

$$D_0 = \int_0^{\phi_M} d\phi\, \Psi^2(\phi) \int_{\phi}^{\phi_0} dx\, \Psi^{-2}(x)$$
$$= \frac{1}{4}\xi t[\ln(8\nu\gamma/t) - (2-C)J] , \qquad (21)$$

$$C_1 = \int_0^{\phi_M} d\phi\, \Psi^2(\phi) \int_{\phi}^{\phi_M} dx\, \Psi^2(x) \int_{\phi}^{x} dy\, \Psi^{-2}(y)$$
$$= \sqrt{\pi}(8\phi_0 e^{\eta})^{-1}(\xi t)^{3/2}$$
$$\times [(2/C)\ln(2\nu\gamma/t) + 2(2-C)J] , \qquad (22)$$

$$D_1 = \int_0^{\phi_M} d\phi \, \Psi^2(\phi) \int_\phi^{\phi_M} dx \, \Psi^2(x) \int_\phi^x dy \, \Psi^{-2}(y)$$

$$\times \int_\phi^{\phi_0} dz \, \Psi^{-2}(z)$$

$$=(2/C)\sqrt{\pi}[32\phi_0 V(0)e^\eta]^{-1}(\xi t)^{7/2}e^{1/t} . \tag{23}$$

These integrals have been carried out by making use of the asymptotic forms of $\Psi(\phi)$ given by Eqs. (14) and (15). In the above expressions, $\gamma = 1.7810\ldots$ is the Euler constant, $C = 2$ in the case of a periodic potential and $C = 1$ in the case of a double-well one, ν is the model-dependent numerical constant given by

$$\nu = \tfrac{1}{2}\xi^{-1}\phi_0^2 e^{2\eta} , \tag{24}$$

ξ and η being defined by Eqs. (3) and (4), and

$$J = \ln(4\gamma/\xi t)$$

$$+2\lim_{\delta\to0}\left[\int_{\phi_0+\delta}^\infty d\phi[2V(\phi)]^{-1/2}+\ln\delta\right] . \tag{25}$$

The constant ν takes values $\nu = 1$, 3, $\tfrac{1}{2}$ for the sine-Gordon, the ϕ^4, and the double-quadratic models.

Substituting Eq. (19) with Eqs. (20)—(23) into Eq. (9), we have[18]

$$\tau_0 = \frac{g^2 T}{m} C \left[\frac{2\nu}{\pi t}\right]^{1/2} e^{-1/t}$$

$$\times \left[1 - C\left[\frac{2\nu}{\pi t}\right]^{1/2} e^{-1/t}\ln\left[\frac{4\nu\gamma}{t}\right]\right] , \tag{26}$$

which gives Eq. (1), the soliton contribution to the free-energy density.

IV. SOLITON-GAS INTERPRETATION

The soliton free energy, Eq. (1), obtained by the transfer-integral method can be interpreted based on a simple soliton-gas picture. We shall first summarize the ideal-gas theory of solitons by Currie et al.[2] and then consider the effect of the interaction between solitons.

We consider solitons and phonons as elementary excitations of the system. At low temperatures ($T \ll M$) the density of solitons are so small that the interaction between solitons can be neglected in the first approximation. Within the ideal-gas approximation the free-energy density of a soliton gas F_s^{id} is given by

$$F_s^{id} = -Tn_0 , \tag{27}$$

where n_0 is the total density of solitons and antisolitons in this approximation. The soliton density n_0 is calculated as

$$n_0 = C \int \frac{dp}{2\pi} e^{-\beta \Delta F(p)} , \tag{28}$$

where $\beta = 1/T$, and $\Delta F(p)$ is the difference of the free energy of the system in the presence of a soliton (or an antisoliton) with momentum p and that in the absence of solitons. The constant C is the "color"[13] of solitons; $C = 1$ for systems with double-well potentials, such as the ϕ^4 model, and $C = 2$ for systems with periodic potentials,

such as the sine-Gordon system. The color is related to the constraint on configuration of solitons and antisolitons:[2] A soliton is always followed by an antisoliton (and vice versa) in the former systems, while there is no restriction on sequence of solitons and antisolitons in the latter systems.

For the class of nonlinear Klein-Gordon systems, $\Delta F(p)$ is given by[5]

$$\Delta F(p) = M + \frac{p^2}{2M} - T \ln(2\nu^{1/2}\beta m) \tag{29}$$

in the "nonrelativistic" limit ($p \ll M$), where ν is the constant given by Eq. (24). The last term of Eq. (29) represents the change in phonon free energy due to the interaction with the soliton. Substituting Eq. (29) into Eq. (28), we have

$$n_0 = Cm \left[\frac{2\nu}{\pi t}\right]^{1/2} e^{-1/t} . \tag{30}$$

Equation (27) with the soliton density n_0 given above yields the leading term of Eq. (1) correctly.

Now we consider the effect of the interaction between solitons. Strength of the interaction decreases exponentially at large distances $|r| \gg m^{-1}$. The potential energy $U(r)$ may be evaluated by examining motion of solitons[19] or by calculating energy of periodic solutions (soliton lattices and "cnoidal waves"[20]). Both of them give the same result:

$$U(r) = \pm 4\nu M e^{-m|r|} \tag{31}$$

for $|r| \gg m^{-1}$. The upper sign is for soliton-soliton and antisoliton-antisoliton interactions, and the lower sign for a soliton-antisoliton interaction. We note that the constant ν is the same as the one appearing in the entropy term of Eq. (29), which comes from the soliton-phonon interaction.

If scatterings of solitons are elastic, they can be described by the "position shift" Δ. Trajectories of solitons (antisolitons) in soliton-soliton and soliton-antisoliton scatterings are schematically shown in Fig. 1, where definition of Δ is given. The quantity Δ may be interpreted
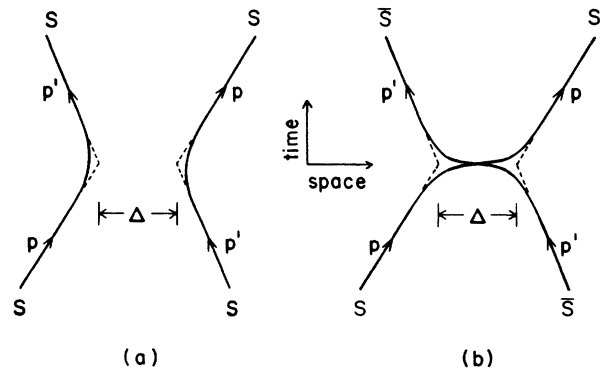

FIG. 1. Definition of the position shift Δ in (a) soliton-soliton (S-S) and (b) soliton-antisoliton (S-$\bar{S}$) scatterings. Solid lines are trajectories of solitons (antisolitons).

as an effective "size" of the soliton in collision, which differs from the usual definition of the soliton size $(\sim m^{-1})$ determined from the waveform of a soliton. In the low-energy limit $(p \ll M)$ Δ is insensitive to details of the interaction at short distances. Elementary calculation of the two-body problem with the potential (31) in classical mechanics gives

$$\Delta(p,p') = 2m^{-1}\ln(2v^{1/2}M / |p - p'|) \qquad (32)$$

for $p,p' \ll M$, where p and p' are asymptotic momenta of solitons (antisolitons). This equation is valid for both attractive and repulsive cases.

The position shift Δ determines the change in the "density of states" in the momentum space due to the interaction.[11,21] The second virial coefficient B in the free energy of a soliton gas is calculated from the position shift Δ as

$$B = \int dp\, dp'\, \Delta(p,p')P(p)P(p')$$
$$= m^{-1}\ln(4v\gamma/t) , \qquad (33)$$

where γ is the Euler constant, and

$$P(p) = (2\pi MT)^{-1/2}\exp(-p^2/2MT)$$

is the momentum distribution function of solitons in the ideal-gas approximation. The free-energy density F_s and the total density n of solitons and antisolitons are given by

$$F_s = -Tn_0(1 - Bn_0) , \qquad (34)$$

$$n = n_0(1 - 2Bn_0) \qquad (35)$$

in the second virial approximation. Substituting Eqs. (30) and (33) into Eq. (34), one finds that Eq. (34) agrees with the transfer-integral result (1). It is apparent from the above analysis that the logarithmic temperature dependence of the second virial coefficient B is attributed to the exponential decay of the interaction potential between solitons at large distances. Therefore this logarithmic behavior should be quite general whenever the soliton tail decays exponentially in space.

V. CONCLUDING REMARKS

The following argument may help to understand the role of the position shift Δ of solitons in thermodynamics

of a soliton gas. The pressure P_s of the soliton gas is given by $P_s = -F_s/T$, since the chemical potential of soliton is zero. From Eqs. (34) and (35), we get the equation of state for the soliton gas

$$P_s(L - BN) = NT , \qquad (36)$$

where L is the size of the system and $N = Ln$ is the total number of solitons and antisolitons. Comparing Eq. (36) with the equation of state for an ideal gas, we can interpret the factor $L - BN$ in Eq. (36) as an effective size or a free volume of the system. This is consistent with the interpretation given in the preceding section that Δ is an effective size of soliton; B is interpreted as the "average size" of solitons as seen from Eq. (33).

To derive Eqs. (34) and (35) we have assumed that soliton scatterings are elastic. However, this is true only for integrable systems (soliton systems in the mathematical sense). Only the sine-Gordon system is an integrable system in the nonlinear Klein-Gordon family. In general, solitons lose or gain their energies in the form of "radiation" (phonon) during their collisions (inelastic scatterings) in nonintegrable systems. Sometimes creation and annihilation of soliton-antisoliton pairs occur. These processes are always accompanied by emissions and absorptions of phonons. Therefore it is plausible that the inelastic scattering of solitons and the creation and annihilation processes contribute to the higher-order terms in t of the second virial term; the elastic scattering is adequate to account for the leading order term in t of the second virial coefficient (presumably, the higher-order virial coefficients also). If this is the case the higher-order calculation of the second virial coefficient will reveal the difference between integrable and nonintegrable systems in statistical mechanics.

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[1]For review, see, for example, A. R. Bishop, J. A. Krumhansl, and S. E. Trullinger, Physica 1D, 1 (1980); *Solitons and Condensed Matter Physics*, edited by A. R. Bishop and T. Schneider (Springer, Berlin, 1978); *Physics in One Dimension*, edited by J. Bernasconi and T. Schneider (Springer, Berlin, 1981).

[2]J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B 22, 477 (1980).

[3]D. J. Scalapino, M. Sears, and R. A. Ferrell, Phys. Rev. B 6, 3409 (1972).

[4]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B 11, 3535

(1975).

[5]R. M. DeLeonardis and S. E. Trullinger, Phys. Rev. B 22, 4558 (1980).

[6]See also, K. Sasaki, Prog. Theor. Phys. 67, 464 (1982).

[7]K. Maki and H. Takayama, Phys. Rev. B 20, 3223 (1979); 20, 5009 (1979).

[8]M. Fowler and X. Zotos, Phys. Rev. B 24, 2634 (1981); 25, 5860 (1982); 26, 1430 (1982); 26, 2519 (1982).

[9]M. Imada, K. Hida, and M. Ishikawa, Phys. Lett. 90A, 79 (1982); J. Phys. C 16, 35 (1983).

[10]K. Sasaki and T. Tsuzuki, J. Magn. Magn. Mater. 31-34, 1283

(1983).

[11]K. Sasaki, Prog. Theor. Phys. **70**, 593 (1983); **71**, 1169 (1984).

[12]K. Maki, Phys. Rev. B **32**, 3075 (1985).

[13]T. Miyashita and K. Maki, Phys. Rev. B **31**, 1836 (1985).

[14]R. M. DeLeonardis and S. E. Trullinger, Phys. Rev. B. **27**, 1867 (1983).

[15]For convenience, the phase of the sine-Gordon potential is shifted by π compared with the standard one.

[16]The effect of the lattice discreteness is examined by S. E. Trullinger and K. Sasaki (unpublished) and by M. Croitoru, D. Grecu, A. Visinescu, and V. Cionga (unpublished).

[17]K. Sasaki, Prog. Theor. Phys. **68**, 411 (1982).

[18]We note that the contribution form the second term in Eq. (20) is cancelled by the one from D_1, and that the terms proportional to J in D_0 and C_1 cancel each other.

[19]J. Rubinstein, J. Math. Phys. **11**, 258 (1970).

[20]D. J. Korteweg and G. de Vries, Philos. Mag. **39**, 422 (1985).

[21]K. Sasaki, Phys. Rev. B **33**, 2214 (1986).