Classical limit of sine-Gordon thermodynamics using the Bethe ansatz

Michael D. Johnson, Niu-Niu Chen, and Michael Fowler
Department of Physics, University of Virginia, McCormick Rd., Charlottesville, Virginia 22901
(Received 27 June 1986)

We use the quantum Bethe ansatz method to compute the free energy of the sine-Gordon model in the classical limit. In this limit the number of breathers, and hence the number of coupled integral equations to be solved, diverges. By linearizing the breather mass spectrum and phase shifts, extending a method of Maki, we can reduce the breather ladder to anharmonic phonons. The divergent set of integral equations is reduced to only two, for interacting phonons and solitons. We solve these equations iteratively to give the free energy in a double series in the temperature t and the soliton density $e^{-1/t}$ which agrees to high order with classical transfer integral results.

I. INTRODUCTION

The study of the statistical mechanics of soliton-bearing systems has come a long way since the pioneering work of Krumhansl and Schrieffer.[1] A particularly useful model is the sine-Gordon (SG) Hamiltonian,[2-4] which is believed to be a reasonable representation of various quasi-one-dimensional physical systems.[5] Many of these are classical, or nearly so, but possible quantum examples include spin chains in magnetic fields.[6-12] Furthermore, the SG system is an excellent testing ground for techniques devised to analyze soliton-bearing systems. For these reasons, the SG model, in both its classical and quantum formulations, has been extensively studied over the last few years. The purely classical system has been rather completely analyzed by transfer-integral methods,[13-17] which have yielded asymptotic series for the free energy and some correlation functions. Semiclassical methods include the ideal-gas phenomenologies[18-21] and the steepest descent analysis of the path integral formulation.[22-27] For the truly quantum system these methods are inadequate, but a mathematically precise technique, the Bethe ansatz (BA),[28-37] exists which in principle can be used to find the free energy to any desired accuracy. In practice, however, it is quite difficult to extract results from the BA, and attempts to link up the quantum regime with the classical have only succeeded to lowest order in the free-energy expansion.[38]

In the present paper we demonstrate that the quantum Bethe ansatz method can in fact be taken to the classical limit and used to find the free energy of the classical sine-Gordon system very accurately. (These results have been reported in summary in Ref. 39.) Our results agree with the recent classical transfer-integral work of Sasaki and Tsuzuki,[16,17] and in fact are no more difficult to derive than theirs. It turns out that in the classical limit the BA method gives two coupled thermodynamic equations, for phonons and solitons, which are exactly of the form derived from ideal-gas phenomenologies. Thus we have been able to tie together three approaches to the statistical mechanics of the sine-Gordon model in the classical limit: the transfer-integral method, ideal-gas phenomenology, and the Bethe ansatz. Very recently, Bullough, Timonen, and co-workers reported that application of Floquet theory to the classical sine-Gordon system leads to the same pair of integral equations we derive in this paper. Using this approach, they independently derived the free-energy expression we present here.[40,41]

The technical difficulty of taking the classical limit of the BA thermodynamic analysis is that it leads to a divergent number of coupled integral equations. In the standard fermionic formulation of sine-Gordon BA thermodynamics, for the special values of coupling $\mu=(1-n^{-1})\pi$, the complete set of excitations consists of the soliton, antisoliton, and $n-2$ breathers (soliton-antisoliton bound states) of different allowed rest energies. The BA thermodynamic analysis is written in terms of a set of functions $\eta_j(\alpha)$ which are the local ratio of empty to filled states for the jth excitation at a point in momentum space parametrized by α (the rapidity).[32] The local available density of states for each excitation depends via the well-known BA phase shifting effect on the distribution of all the other excitations. This, together with minimization of the free-energy functional, leads to a set of n coupled integral equations for the n density functions $\eta_j(\alpha)$. In the zero-charge sector, the local soliton and antisoliton densities are equal and the number of equations can be reduced by one. Once these equations are solved for the η_j's, it is straightforward to find the free energy. The BA solution of the SG thermodynamics is detailed in Sec. II. In the classical SG limit the number of different allowed breather rest energies goes to infinity, and hence so does the number of coupled integral equations for their density functions η_j. The integral equations with a large momentum-space cutoff can be solved numerically to high accuracy for n up to about 50 (and for $n\sim 250$ with a low cutoff[35]). The numerical solution is not really satisfactory for comparison with classical transfer integral results, because the latter are only valid in a temperature range far above the phonon (lowest breather) mass but far below the soliton mass. For n of order 50, the ratio of soliton to phonon mass is only about 15.

To handle the classical limit successfully, one must somehow transform away from this diverging number of coupled integral equations. The basic strategy for accomplishing this is rooted in the well-known boson-fermion duality of the sine-Gordon system. In particular, the low-temperature thermodynamic properties of the system are dominated by the most tightly bound soliton-antisoliton bound states, the lowest breathers in the fermion picture. These are easier to understand in the boson, or phonon, representation. In this picture, the lowest energy breather is a single phonon, the next one up (in rest mass) is a bound state of two phonons, the next of three phonons, etc. Furthermore, in the classical limit the binding energies of these states go to zero faster than the phonon rest mass, so, in the limit of large n, the lowest states form a ladder of equally spaced rest masses $m, 2m, 3m, \ldots$ (where of course m is of order $1/n$).

It is instructive to consider the Klein-Gordon (KG) limit,[34] in which we take n to infinity but keep the phonon mass and the temperature fixed. In this limit, the soliton mass goes to infinity and the SG Hamiltonian reduces to the KG Hamiltonian, describing noninteracting massive bosons. Yet the BA thermodynamic analysis of this system appears quite complicated—it is written in terms of the infinite ladder of breather states with equally spaced masses $m, 2m, 3m, \ldots$ mentioned above. However, in the KG limit these breathers are formal constructs rather than physical entities. They provide a way for the quasi-fermionic BA formulation to accommodate many bosons in the same quantum state. In fact, as is shown in Sec. III, the infinite set of integral equations in this limit becomes a set of algebraic equations which can be solved analytically to give the free energy of the free boson gas.

The key to our approach here is that this analytical reduction of the BA breather ladder in the rather trivial KG limit can be generalized to the true classical limit, where the phonon mass goes to zero while the temperature and the soliton mass remain finite. The first step in this direction was taken by Maki.[38] He considered a low-temperature semiclassical situation, in which the number of distinct breather states diverged, but only the first few of them were significantly thermally occupied. These lowest members of the ladder of breathers are almost equally spaced in energy and are close to the KG limit discussed above, so he replaced them by a non-self-interacting boson gas. At the same time, he kept the soliton mass finite and retained the soliton-soliton and soliton-breather (or soliton-phonon) phase shift terms in the analysis. By this method he was able to sum up the contributions to the BA thermodynamic equations from the ladder of breathers and replace it with a single phonon density. This led to a set of just two coupled equations, for the phonon density and the soliton density (in the zero-charge sector). This approach successfully gave the leading term in the free energy from the phonons (the free phonon term), the solitons ($t^{1/2}e^{-1/t}$), the soliton-soliton interactions ($e^{-2/5}\ln t$), etc.

In the present work, we extend Maki's analysis to include the phonon-phonon interactions. In the classical limit, we find the analysis gives the anharmonic terms in the free energy in nearly exact agreement, to very high order, with classical transfer integral results. This, the main substance of our work, is presented in Sec. IV and Appendixes B and C.

There is another kind of boson-fermion duality in the BA besides that discussed above. For example, the δ-function Bose gas,[42–44] the prototype BA system, is ordinarily treated using the BA in a fermionic fashion. As was recently pointed out by Wadati,[45] this analysis can be recast in a bosonic fashion which changes no final result but in some ways is more natural. In Sec. V we reconsider our transformation of the BA thermodynamics in the classical limit from this point of view. In this section we also connect our work to ideal gas phenomenologies. Section VI is a discussion of our results.

II. BETHE ANSATZ THERMODYNAMICS

The quantum sine-Gordon (SG) model is described by the Hamiltonian ($\hbar = c = 1$)

$$\mathscr{H} = \tfrac{1}{2} \int dx \left[\phi_t^2 + \phi_x^2 + \frac{2m^2}{g^2} {:}[1-\cos(g\phi)]{:} \right] , \tag{2.1}$$

where ϕ is a real scalar field in $1+1$ dimensions obeying boson commutation relations, m is the boson (phonon) mass, the colons represent normal ordering, and g is the SG coupling constant. In this section we summarize the solution for the thermodynamics of the quantum SG (or equivalently the massive Thirring model[46]) derived using the Bethe ansatz (BA).[31–33]

The excitations in the BA analysis of the quantum SG system are bound-state-type combinations known as strings, each of which consists of a string of complex momenta; all string lengths corresponding to normalizable wave functions are allowed. For a general value of the coupling parameter μ (where $\mu = \pi - g^2/8$), an infinite number of different string lengths are allowed, and hence the thermodynamic equations form an infinite set. However, for the special values $\mu = (1-n^{-1})\pi$, where n is an integer, there are only n distinct string lengths allowed and these correspond exactly to the excitation (breathers, solitons, and antisolitons) found by Dashen, Hasslacher, and Neveu[3] (DHN) using semiclassical quantization. The shortest $n-2$ string lengths in the BA analysis represent the DHN breather spectrum, the $(n-1)$ string is a soliton, and holes in the Dirac sea (which lies along the $\mathrm{Im}\beta = \pi$ line) correspond to antisolitons.

In the BA approach to thermodynamics, the free energy is written as a functional of the local densities of occupied (ρ_j) and unoccupied ($\tilde{\rho}_j$) j-string states in rapidity space. Minimizing the free energy with respect to local density variations, subject to the nonlocal BA boundary condition equations, yields a set of coupled integral equations for the ratios

$$\eta_j(\beta) = \tilde{\rho}_j(\beta)/\rho_j(\beta) , \tag{2.2}$$

where β is the rapidity. For the special values of coupling $\mu = (1-n^{-1})\pi$, the phase shifts between a hole and any excitation equals the phase shift between an $(n-1)$ string and the same excitation. In the zero-charge sector, moreover, the local hole and $(n-1)$-string densities are equal; and so, when $\mu = (1-n^{-1})\pi$, the BA thermodynamic equations can be written as the $n-1$ equations:[32,37]

$$\ln\eta_j(\alpha)=\frac{M_j}{T}\cosh\alpha+\frac{1}{2\pi}\sum_{k=1}^{n-2}\int_{-\infty}^{\infty}d\alpha'\theta'_{jk}(\alpha'-\alpha)\times\ln[1+\eta_k^{-1}(\alpha')]+\frac{2}{2\pi}\int_{-\infty}^{\infty}d\alpha'\theta'_{js}(\alpha'-\alpha)\times\ln[1+\eta_s^{-1}(\alpha')],\quad j=1\text{ to }n-2 \tag{2.3a}$$

$$\ln\eta_s(\alpha)=\frac{M}{T}\cosh\alpha+\frac{1}{2\pi}\sum_{k=1}^{n-2}\int_{-\infty}^{\infty}d\alpha'\theta'_{ks}(\alpha'-\alpha)\times\ln[1+\eta_k^{-1}(\alpha')]+\frac{2}{2\pi}\int_{-\infty}^{\infty}d\alpha'\theta'_{ss}(\alpha'-\alpha)\ln[1+\eta_s^{-1}(\alpha')]\ , \tag{2.3b}$$

where $\alpha=\pi\beta/2\mu$ is the dressed rapidity. The subscripts $j=1,2,\ldots,n-2$ correspond to breathers in the DHN spectrum, and s means solitons or antisolitons [$(n-1)$ strings or holes in the BA language]. The last term in each of Eqs. (2.3) is the sum of the equal contributions of both solitons and antisolitons [i.e., $(n-1)$ strings plus holes]—hence the factor of 2. The breather mass spectrum is related to the soliton mass M by[3,32]

$$M_j=2M\sin\left[\frac{\pi}{2}\frac{j}{n-1}\right],\quad j=1,2,\ldots,n-2\ . \tag{2.4}$$

The functions $\theta(\alpha)$ are the dressed phase shifts between excitations separated by a relative dressed rapidity α, and $\theta'(\alpha)\equiv d\theta/d\alpha$. The breather-breather phase shifts are given by[32,37]

$$\theta_{jk}(\alpha)=f_{jk}(\alpha),\quad j,k=1,2,\ldots,n-2 \tag{2.5}$$

where

$$f_{jk}(\alpha)=\theta(\alpha,j+k)+\theta(\alpha,|j-k|)+2\sum_{l=1}^{\min(j,k)-1}\theta(\alpha,j+k-2l) \tag{2.6a}$$

and

$$\theta(\alpha,j)=-i\ln\left[\frac{\sinh\alpha-i\sin\left[\dfrac{\pi}{2}\dfrac{j}{n-1}\right]}{\sinh\alpha+i\sin\left[\dfrac{\pi}{2}\dfrac{j}{n-1}\right]}\right]. \tag{2.6b}$$

The derivatives of the breather-soliton and soliton-soliton phase shifts are, respectively,[37]

$$\theta'_{js}(\alpha)=\int_{-\infty}^{\infty}dk\,e^{-i\alpha k}\frac{\cosh\left[\dfrac{\pi}{2}\dfrac{k}{n-1}\right]\sinh\left[\dfrac{\pi}{2}\dfrac{jk}{n-1}\right]}{\sinh\left[\dfrac{\pi}{2}\dfrac{k}{n-1}\right]\cosh\left[\dfrac{\pi k}{2}\right]}\ , \tag{2.7a}$$

$$\theta'_{ss}(\alpha)=\tfrac{1}{2}\int_{-\infty}^{\infty}dk\,e^{-i\alpha k}\frac{\sinh\left[\dfrac{\pi}{2}\dfrac{n-2}{n-1}k\right]}{\sinh\left[\dfrac{\pi}{2}\dfrac{k}{n-1}\right]\cosh\left[\dfrac{\pi k}{2}\right]}\ . \tag{2.7b}$$

(The form of these phase shifts and the thermodynamic equations are discussed in Appendix A.)

Given the η's which solve (2.3), the free energy per unit length is given by[32]

$$F=-\frac{T}{2\pi}\sum_{j=1}^{n-2}\int_{-\infty}^{\infty}M_j\cosh\alpha\ln(1+\eta_j^{-1})d\alpha-\frac{2T}{2\pi}\int_{-\infty}^{\infty}M\cosh\alpha\ln(1+\eta_s^{-1})d\alpha \tag{2.8}$$

and the local density of jth breathers per unit length is

$$\rho_j(\alpha)=\frac{T^2}{2\pi}\frac{\partial}{\partial T}\ln[1+\eta_j^{-1}(\alpha)] \tag{2.9}$$

with an identical expression for ρ_s.

III. KLEIN-GORDON LIMIT

The analytic structure which makes it possible to reduce Eqs. (2.3) to just two coupled equations in the classical limit is most easily seen in a related but simpler case, the limit of noninteracting phonons.[34] In this limit the soliton mass M is allowed to become infinite as the coupling parameter $\mu\to\pi$, while the lightest breather's mass M_1 and the temperature are held fixed. Then only breathers with relatively small masses are thermally excited and the solitons can be neglected entirely. We choose to take μ to π through the sequence of special values $\mu=(1-n^{-1})\pi$ by letting $n\to\infty$. From (2.4) as $n\to\infty$ the masses of low-lying breathers become uniformly spaced,

$$M_j\approx jm,\quad m=M\pi/n \tag{3.1}$$

and from (2.5) and (2.6) the breather-breather phase shifts become step functions:

$$\theta_{jk}(\alpha)=2\pi[2\min(j,k)-\delta_{jk}]H(\alpha)\ , \tag{3.2}$$

where

$$H(\alpha)=\begin{cases}0, & \alpha<0\\ \tfrac{1}{2}, & \alpha=0\\ 1, & \alpha>0\ .\end{cases} \tag{3.3}$$

Thus as $n\to\infty$ the thermodynamic equations (2.3) become an algebraic set,

$$\ln\eta_j=jE/T+\sum_{k=1}^{\infty}[2\min(j,k)-\delta_{jk}]\times\ln(1+\eta_k^{-1}),\quad j=1\text{ to }\infty \tag{3.4}$$

where

$$E(\alpha)=m\cosh\alpha\ , \tag{3.5}$$

which can be solved algebraically to give[34]

$$1+\eta_j^{-1}=\frac{\sinh^2[(j+1)E/2T]}{\sinh(jE/2T)\sinh[(j+2)E/2T]}\ . \tag{3.6}$$

By directly using (3.6), or more simply by considering (3.4) as $j\to\infty$, one finds

$$\sum_{j=1}^{\infty} j\ln(1+\eta_j^{-1})=-\ln(1-e^{-E/T})\ . \tag{3.7}$$

Combined with (2.8) and (3.1), this gives

$$F=\frac{T}{2\pi}\int_{-\infty}^{\infty} d\alpha E(\alpha)\ln(1-e^{-E/T}) \tag{3.8}$$

which is just the free energy of a noninteracting relativistic phonon gas of mass m.

This result could have been anticipated—in this limit the sine-Gordon equation becomes the Klein-Gordon (KG) equation, and (3.8) describes the noninteracting KG phonons. Frequently the lowest ($j=1$) breather in the BA analysis is thought to represent a phonon, which we call the "BA phonon." It is important to realize that the KG and BA phonons are different physical objects. The KG phonons do not interact and many of them can occupy a single momentum state. The BA phonons do interact and can bind to form the breather states; and only one BA phonon (or any other breather type) can exist in any momentum state. The linear mass spectrum (3.1), as well as comparison of (3.7) and (2.9), show that in this limit the jth breather is effectively equivalent to j KG phonons—more precisely, the jth breather represents a "bound state" of j KG phonons with zero binding energy. The multiple occupancy of a momentum state by KG phonons is represented in the BA picture by breathers of many different types at the same momentum. Thus in the infinite-n and infinite-soliton mass limit, the entire ladder of BA breathers combine to represent the KG phonons.

IV. CLASSICAL SG LIMIT: SOLITONS AND ANHARMONIC PHONONS

The classical SG limit consists of taking μ to π while holding the soliton mass and the temperature fixed, in which case the phonon mass goes to zero. In contrast to the related KG limit discussed in Sec. III, in the classical limit the entire breather spectrum and also the solitons are thermally excited and must be retained in the thermodynamic analysis. In this section we will demonstrate that the breather spectrum can again be reduced to a single phonon contribution in this limit, so that the thermodynamic equations can be reduced to just two—for phonons and solitons. The procedure we follow is quite similar to a partial analysis of this limit due to Maki.[38]

It is convenient to approach the classical limit through a sequence of the special values $\mu=(1-n^{-1})\pi$ by taking $n\to\infty$. Then in the classical limit the number of coupled integral equations (2.3) becomes infinite. Since the free energy is analytic in μ, any other approach to this limit will of course give the same result. For instance, if one sets $\mu=(1-n^{-1}+\epsilon)\pi$ (ϵ irrational), then the thermodynamic equations form an infinite set even for finite n; however, as $\epsilon\to 0$ all but $n-1$ of the equations become algebraic and the infinite set becomes equivalent to (2.3).[37]

As $n\to\infty$, the lower breather masses are approximately uniformly spaced, as in (3.1):

$$M_j\approx jm\ ,\ \ j\ll n \tag{4.1}$$

where the phonon mass $m=M\pi/n$ vanishes as n^{-1} since the soliton mass M is fixed. For large n, the soliton-soliton and breather-soliton phase shift derivatives (2.7) take the form[38]

$$\theta'_{ss}(\alpha)\approx\frac{n}{\pi}\ln\left[\frac{\cosh\alpha+1}{\cosh\alpha-1}\right]\ , \tag{4.2}$$

$$\theta'_{js}(\alpha)\approx 2j\,\mathrm{sech}\alpha\ ,\ \ j\ll n\ . \tag{4.3}$$

The breather-breather phase shifts are given in (2.5) in terms of a function $\theta(\alpha,j)$ defined, except for a choice of branch, by Eq. (2.6b). The SG thermodynamic equations (2.3) were derived assuming $\theta(\alpha,j)$ continuous, and we can choose

$$\theta(\alpha,j)=\begin{cases}2\tan^{-1}(\sinh\alpha/a_j)+\pi, & j\neq 0\ ,\\ 0, & j=0\end{cases} \tag{4.4}$$

where

$$a_j=\sin\left[\frac{\pi}{2}\frac{j}{n-1}\right] \tag{4.5}$$

and where $\tan^{-1}$ means the principal branch: $|\tan^{-1}x|\leq\pi/2$. In the limit $n\to\infty$, $\theta(\alpha,j)$ goes to a step function and so it is natural to write (4.4) as a sum of two discontinuous pieces:

$$\theta(\alpha,j)=2\pi H(\alpha)-2\tan^{-1}\left[\frac{a_j}{\sinh\alpha}\right],\ \ j\neq 0 \tag{4.6}$$

where the step function $H(\alpha)$ is defined in (3.3) and again $\tan^{-1}$ means the principal branch. (See Sec. V for a discussion of this point.) In any integral involving $\theta(\alpha,j)$, the second term in (4.6) can be written as a principal part integral as $n\to\infty$:

$$2\tan^{-1}\left[\frac{a_j}{\sinh\alpha}\right]\approx\frac{j\pi}{n}P\frac{1}{\sinh\alpha},\ \ j\ll n\ . \tag{4.7}$$

Finally, inserting (4.6) and (4.7) into (2.5) and (2.6) gives the following expression for the phase shift between low-lying breathers as $n\to\infty$:

$$\theta_{jk}(\alpha)\approx 2\pi[2\min(j,k)-\delta_{jk}]H(\alpha)-jk\frac{2\pi}{n}P\frac{1}{\sinh\alpha},\ \ j,k\ll n\ . \tag{4.8}$$

In the approximations (4.1) and (4.3), the mass of the jth breather and its phase shift with solitons are proportional to j, which is consistent with interpreting the jth breather as representing j physical phonons (as in Sec. III). Similarly, the n^{-1} term in (4.8) represents an interaction between j physical phonons in one breather and k in another. In Sec. III we distinguished between the "BA phonon" (really just the lowest breather) and the physical KG phonon which was noninteracting. Now the physical phonons are anharmonic (i.e., they do interact with one another), and we call them the SG phonons. Although the expressions (4.1), (4.3), and (4.8) are valid only for $j \ll n$, we will use them for all breathers. This approximation should accurately include the contributions of the soliton and SG phonon to the thermodynamics, while perhaps neglecting extra nonphonon contributions (if any exist) from the heavy breathers. This is discussed further in Sec. VI.

If we use the equally spaced breather mass spectrum (4.1) and the large-n approximations for the phase shifts (4.2), (4.3), and (4.8), the BA thermodynamic equations (2.3) become

$$\ln\eta_j(\alpha)=jw(\alpha)+\sum_{k=1}^{n-2}[2\min(j,k)-\delta_{jk}]\times\ln(1+\eta_k^{-1}),\quad j=1 \text{ to } n-2 \tag{4.9}$$

$$\ln\eta_s(\alpha)=\frac{M}{T}\cosh\alpha+\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{d\alpha'}{\cosh(\alpha'-\alpha)}\times\sum_{k=1}^{n-2}k\ln[1+\eta_k^{-1}(\alpha')]+\frac{n}{\pi^2}\int_{-\infty}^{\infty}d\alpha'\ln\left|\frac{\cosh(\alpha'-\alpha)+1}{\cosh(\alpha'-\alpha)-1}\right|\times\ln[1+\eta_s^{-1}(\alpha')]\,, \tag{4.10}$$

where

$$w(\alpha)=\frac{m}{T}\cosh\alpha+\frac{1}{n}P\int_{-\infty}^{\infty}\frac{d\alpha'}{\sinh(\alpha'-\alpha)}\frac{\partial}{\partial\alpha'}\times\sum_{k=1}^{n-2}k\ln[1+\eta_k^{-1}(\alpha')]+\frac{2}{\pi}\int_{-\infty}^{\infty}\frac{d\alpha'}{\cosh(\alpha'-\alpha)}\ln[1+\eta_s^{-1}(\alpha')]\,. \tag{4.11}$$

The study of the classical limit per se was begun by Maki, whose approach we have closely followed.[38] He used the approximations (4.1), (4.2), and (4.3), but neglected the $1/n$ term in (4.8). This leads to the omission of the second term on the right-hand side of (4.11), which represents the interaction between SG phonons. Maki's analysis resulted in a gas of solitons and harmonic KG-type phonons, whereas the present work gives the anharmonic SG phonons.

The structure of the breather equations (4.9) is the same as in the noninteracting phonon limit discussed in Sec. III [Eq. (3.4)], and we can use a similar analysis here to reduce the $n-2$ breather equations to a single equation for the SG phonons. It is important to realize that this structure depends crucially upon having the jth breather's mass and phase shifts proportional to j, which, as discussed above, is consistent with interpreting it as j SG phonons.

We proceed by formally solving Eqs. (4.9) for η_j in terms of w. Then, replacing the terms in (4.10) and (4.11) that depend on η_k by functions of w, we will be left with only two coupled equations. The solution of (4.9) follows the lines of the analysis of the noninteracting phonon limit.[34] Subtracting Eq. (4.9) for j from that for $j+1$, and repeating the process, one gets a set of difference equations,

$$2\ln\eta_j=\ln(1+\eta_{j+1})+\ln(1+\eta_{j-1}),\quad j=2 \text{ to } n-3 \tag{4.12}$$

which is solved by [cf. (3.6)]

$$1+\eta_j^{-1}=\frac{\sinh^2[(j+1)\lambda]}{\sinh j\lambda\,\sinh[(j+2)\lambda]}\,, \tag{4.13}$$

where $\lambda(\alpha)$ is related to $w(\alpha)$ by

$$w(\alpha)=2\ln\left|\frac{\sinh(n\lambda)}{\sinh[(n-1)\lambda]}\right|\,. \tag{4.14}$$

Notice that η_k only enters (4.10) and (4.11) in a sum over $k\ln(1+\eta_k^{-1})$. By considering (4.9) for $j=n-2$ and using (4.13), one finds

$$\sum_{k=1}^{n-2}k\ln(1+\eta_k^{-1})=-\ln(1-e^{-w})-\ln\left|\frac{\sinh(n\lambda)}{\sinh[(2n-1)\lambda]}\right|-\tfrac{1}{2}(n-1)w\,. \tag{4.15a}$$

In the limit $n\to\infty$, w vanishes as n^{-1} [see (4.11) and Appendix B]; hence λ also vanishes as n^{-1}, and it is not difficult to show, using (4.14), that (4.15a) becomes [cf. (3.7)]

$$\sum_{k=1}^{n-2}k\ln(1+\eta_k^{-1})=-\ln(1-e^{-w})+0(e^{-\pi/t})+O(n^{-1})\,, \tag{4.15b}$$

where $t=T/M$ is a reduced temperature. The $e^{-\pi/t}$ term in (4.15b) is an artifact, a consequence of linearizing the breather mass spectrum as in (4.1) so that heavy breathers have masses approaching πM rather than $2M$. We shall neglect this term (see Sect. VI).

Plugging (4.15b) into (4.10) and (4.11) we get, for large n, the two coupled equations

$$\ln\eta_p(\alpha)=\frac{m}{T}\cosh\alpha-\frac{1}{n}P\int_{-\infty}^{\infty}\frac{d\alpha'}{\sinh(\alpha'-\alpha)}\times\frac{\partial}{\partial\alpha'}\ln[1-\eta_p^{-1}(\alpha')]+\frac{2}{\pi}\int_{-\infty}^{\infty}\frac{d\alpha'}{\cosh(\alpha'-\alpha)}\ln[1+\eta_s^{-1}(\alpha')]\,, \tag{4.16a}$$

$$\ln\eta_s(\alpha)=\frac{M}{T}\cosh\alpha-\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{d\alpha'}{\cosh(\alpha'-\alpha)}\times\ln[1-\eta_p^{-1}(\alpha')]+\frac{n}{\pi^2}\int_{-\infty}^{\infty}d\alpha'\ln\left|\frac{\cosh(\alpha'-\alpha)+1}{\cosh(\alpha'-\alpha)-1}\right|\times\ln[1+\eta_s^{-1}(\alpha')]\,, \tag{4.16b}$$

where

$$\ln\eta_p(\alpha)=w(\alpha) \tag{4.17}$$

and the subscript p means phonons. Thus the infinite set of BA thermodynamic equations in the classical limit has been reduced to just two equations, for interacting phonons and solitons. It is interesting to note that the form of Eqs. (4.16) is exactly what one would expect from a gas phenomenology (see Sec. V).

Given the solutions η_p and η_s of (4.16), the free energy can be written, using (2.8), (4.1), (4.15b), and (4.17),

$$F(T)=\frac{mT}{2\pi}\int_{-\infty}^{\infty}d\alpha\cosh\alpha\ln(1-\eta_p^{-1}) -\frac{MT}{\pi}\int_{-\infty}^{\infty}d\alpha\cosh\alpha\ln(1+\eta_s^{-1}) . \tag{4.18}$$

The solution of Eqs. (4.16) as $n\to\infty$, for $T\ll M$, takes the form of a double series in $e^{-1/t}$ and t, where

$$t=T/M . \tag{4.19}$$

The calculation is somewhat lengthy, and is summarized in Appendix B. We find the following free energy (per unit length) in the classical limit:

$$\begin{aligned}F=F_{\rm non}&-mM[\tfrac{1}{4}t^2+\tfrac{1}{8}t^3+\tfrac{3}{16}t^4+\tfrac{53}{128}t^5+\tfrac{297}{256}t^6+O(t^7)]\\&-2mM\left[\frac{2t}{\pi}\right]^{1/2}e^{-1/t}[1-\tfrac{7}{8}t-\tfrac{59}{128}t^2-\tfrac{897}{1024}t^3-\tfrac{75005}{32768}t^4+O(t^5)]\\&+\frac{8}{\pi}mMe^{-2/t}\left\{\ln\left[\frac{4\gamma}{t}\right]-\frac{5}{4}t\left[\ln\left[\frac{4\gamma}{t}\right]+1\right]-\frac{1}{32}t^2\left[13\ln\left[\frac{4\gamma}{t}\right]+2\right]+O(t^3)\right\}+O(e^{-3/t}) ,\end{aligned} \tag{4.20}$$

where $F_{\rm non}$ is the free energy of noninteracting phonons given in (3.8) and $C=\ln\gamma=0.577\,215\,66\ldots$ is Euler's constant.

Our results for the free energy agree nearly exactly with the classical transfer integral work of Sasaki and Tsuzuki.[16,17] The noninteracting phonon term $F_{\rm non}$ in our work results from taking an infinite cutoff in momentum space, which leaves some phonon modes unoccupied at any finite temperature even in the classical limit; in the transfer-integral work, a finite cutoff results in a Dulong-Petit term. All of the higher-order terms in (4.20) result from nonlinear behavior—solitons and interactions among phonons and solitons—and agree exactly with the transfer-integral results, except for the $t^2e^{-2/t}$ term, where in large square brackets Sasaki[17] gets $13\ln(4\gamma/t)+4$ (see Sec. VI).

V. FERMIONIC AND BOSONIC PICTURES

Although the physical quantum SG Hamiltonian is a boson system, in the BA formalism, its excitation, the breathers, are quasifermionic—they obey a kind of exclusion principle in that no two breathers of a given size can have the same rapidity. Our above analysis shows that in the classical limit (to the extent that the linearization procedure is accurate), the ladder of quasifermionic breathers can be replaced by interacting bosons. It is illuminating to connect this to a related type of fermionic-bosonic duality which, as was recently pointed out by Wadati, is exhibited by the well-known δ-function Bose gas.[45]

A gas of bosons in one dimension interacting via repulsive δ-function potentials is described by the Hamiltonian

$$\mathscr{H}=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+2c\sum_{i<j}\delta(x_i-x_j) , \tag{5.1}$$

where $c>0$ (repulsive) and N is the number of bosons. The second-quantized form of the above is the nonlinear Schrödinger model,

$$\mathscr{H}=\int dx(\phi_x^\dagger\phi_x+c\phi^\dagger\phi^\dagger\phi\phi) . \tag{5.2}$$

The ground state and excitations of this model were found using the BA by Lieb and Liniger,[42,43] and this was the system analyzed by Yang and Yang[44] in their classic paper introducing the methods of BA thermodynamics. The point of Wadati's work is to emphasize that in the BA solution there is an ambiguity (a choice of branch) in the definition of the phase shift in two-particle scattering, and that it is this choice of branch which leads to either a bosonic or fermionic description of the same physical system.[45]

In the δ-functions Bose gas case, if one chooses the following continuous branch of the phase shift,

$$\Delta(k)=\pi-2\tan^{-1}(k/c),\quad 0\le\Delta\le2\pi \tag{5.3}$$

the quasimomenta k_j in the many-particle wave function satisfy the boundary condition equation

$$k_jL=2\pi I_j+\sum_{i\neq j}\Delta(k_j-k_i),\quad j=1,2,\ldots,N \tag{5.4}$$

where the quantum numbers I_j are integers. Given a set of I_j's, the k_j's are uniquely determined. The BA wave function vanishes when any two k_j's are equal, and the choice of the continuous phase shift (5.3) results in the requirement that all of the I_j's be distinct (as they would be for a system of noninteracting fermions). The ground state is given by a fermionic distribution of the quantum numbers: $I_{j+1}-I_j=1$. This fermionic description of the Bose gas is the choice usually made.[42–44]

On the other hand, as was emphasized by Wadati, one could equally well have chosen the following discontinuous branch of the phase shift (introduced by Thacker[30]),

$$\tilde{\Delta}(k)=2\tan^{-1}(c/k)=\Delta(k)-2\pi H(-k),\quad |\Delta|\le\pi \tag{5.5}$$

where $H(k)$ is the step function defined in (3.3). The boundary condition gives

$$k_jL=2\pi\tilde{I}_j+\sum_{i\neq j}\tilde{\Delta}(k_j-k_i)\ . \tag{5.6}$$

With the discontinuous choice of branch, quantum numbers $\tilde{I}_j$ are allowed to be equal, which is the behavior expected for a system of bosons; and in fact the ground state is given by the bosonic description $\tilde{I}_j=0$. It is easy to see how this comes about—for each $i>j$, $\tilde{\Delta}(k_j-k_i)$ adds an extra -2π onto the right-hand side of (5.6) compared with (5.5); thus $\tilde{I}_j$ must be greater than I_j by one for each filled i greater than j, and for I_j's sequential integers, the $\tilde{I}_j$'s will all be equal.

It should be emphasized that the two approaches give identical states of the system (5.1)—the sets of k's which solve (5.4) and (5.6) are the same, and can be labeled by a set of either I_j's or $\tilde{I}_j$'s. In particular, in the bosonic ground state where all bosons have the same quantum number $\tilde{I}_j=0$, they still all have different k_j's provided the interaction strength is nonzero. The choice of description is just a matter of convenience. In the weakly interacting limit ($c=0$), the bosonic (discontinuous phase shift) picture is more natural—as $c\rightarrow 0$, $\tilde{\Delta}$ vanishes but Δ goes to a step function. On the other hand, in the limit of impenetrable bosons ($c\rightarrow\infty$), the fermionic description is simpler—the wave function in that limit is identical to that for noninteracting fermions except of course for the (-1) factors on permuting particles. Essentially this same analysis of the choice of branch was given for the *XXZ* spin chain by des Cloizeaux and Gaudin many years ago.[47]

Either description—fermionic or bosonic—can also be used to derive the thermodynamics. In the fermionic picture (used by Yang and Yang[44]), each k_j (or equivalently each I_j) is considered a particle state, and in the thermodynamic limit one defines a local density of occupied $[\rho(k)]$ and unoccupied $[\tilde{\rho}(k)]$ states. The density of available states is $\rho+\tilde{\rho}$. Minimizing the free-energy functional with respect to variations in ρ, subject to the BA boundary condition equation (5.4), yields an equation for $\eta=\tilde{\rho}/\rho$:

$$\ln\eta(k)=\frac{1}{T}(k^2-\mu)+\frac{1}{2\pi}\int_{-\infty}^{\infty}dq\,\Delta'(k-q)\ln[1+\eta^{-1}(q)]\,, \tag{5.7}$$

where μ is the chemical potential. The free energy per unit length can then be written as

$$F=\mu D-\frac{T}{2\pi}\int_{-\infty}^{\infty}dk\,\ln(1+\eta^{-1})\ , \tag{5.8}$$

where $D=N/L$.

In the bosonic picture (analyzed by Wadati[45]), more than one k_j can share the same quantum number, and one can define the number of available states in a range dk to be the number of distinct I's which correspond to (one or more) k's in dk. In the thermodynamic limit there will be a density f of available states and a density ρ of occupied k's. An analysis very similar to Yang and Yang's, but with a *bosonic* entropy term, gives the following equation for $\tilde{\eta}=1+f/\rho$:

$$\ln\tilde{\eta}(k)=\frac{1}{T}(k^2-\mu)-\frac{1}{2\pi}\int_{-\infty}^{\infty}dq\,\tilde{\Delta}'(k-q)\times\ln[1-\tilde{\eta}^{-1}(q)]\ . \tag{5.9}$$

The free energy per unit length is

$$F=\mu D+\frac{T}{2\pi}\int_{-\infty}^{\infty}dk\,\ln(1-\tilde{\eta}^{-1})\ . \tag{5.10}$$

The two approaches give the same free energy and the same local density of bosons ρ. Notice that the bosonic thermodynamic equations (5.9) and (5.10) can be derived from the fermionic equations (5.7) and (5.8) by writing Δ in terms of $\tilde{\Delta}$ in the latter, using (5.5), and we find $\tilde{\eta}=1+\eta$.

We now turn to the thermodynamics of the quantum sine-Gordon model, and examine the similarities and differences between this case and Wadati's boson gas. In the language developed above, the SG thermodynamic equations (2.3) are based on a fermionic picture—no two jth breathers can have the same quantum number. As was mentioned in Sec. IV, the thermodynamics derivation was based on the choice of a continuous branch of the phase-shift function $\theta(\alpha,j)$ [Eq. (2.6b)]. For analysis of the classical limit this is an unnatural choice, since as $n\rightarrow\infty$, $\theta(\alpha,j)$ goes to a step function. Like Wadati, we choose a new phase shift branch by subtracting off the step function [cf. (4.6)]:

$$\tilde{\theta}(\alpha,j)=\theta(\alpha,j)-2\pi H(\alpha)=-2\tan^{-1}\left[\frac{a_j}{\sinh\alpha}\right]\ . \tag{5.11}$$

This gives a phase shift discontinuous at the origin but vanishing in the limit of zero coupling. In Sec. IV we transformed the SG thermodynamic equations (2.3) into a bosonic form by writing $\theta(\alpha,j)$ in terms of $\tilde{\theta}(\alpha,j)$, much as (5.7) can be transformed into (5.9) by using (5.5).

Although there is a pleasing similarity between the bosonizations of these two systems, there is also a very important difference: whereas the repulsive δ-function Bose gas can be bosonized for *any value of the coupling* by choosing the discontinuous branch, the bosonization of the SG requires the extra step of taking the classical (zero-coupling) limit. As we shall see, this is because in the SG system the interaction is attractive.

The regime of the SG most closely analogous to Wadati's analysis is given by taking the weak-coupling and nonrelativistic limits of the SG. Then with a fixed number of bosons, the SG Hamiltonian (2.1) becomes, to leading order in the interaction, identical to the ϕ^4 Hamiltonian (5.2) except that now we have a system of *attractive* bosons ($c=-mg^2/8<0$). (The temperature range we are ultimately interested in is far greater than the phonon mass, but the discussion of phase shifts given below generalizes to the physical case.) In the thermodynamic limit, it is well known that such a gas collapses into a single bound state. In the case of the SG, however, higher-order terms in the interaction prevent this from happening, and so the mixed gas of free bosons and bound states occurring at low temperatures is stable for the SG system even though it would be only metastable for the attractive ϕ^4 system. There are several important differences between the attractive boson gas and Wadati's repulsive boson gas.

Consider first the phase shift. For the repulsive case, in the limit of weak coupling the continuous branch becomes a step function. Wadati bosonized by subtracting off this step function. In the attractive case (a limit of the SG, as described above), the phase shift again goes to a step function at zero coupling, but in the opposite direction, and there is a zero-energy bound state. [Note that in this limit $\Delta(k)=\theta(\alpha,2)$.] The existence of bound states makes the attractive case more complicated.

The relationship between k_j values and I_j or $\tilde{I}_j$ quantum numbers is tricky in the attractive case, because it depends on phase-shift sheet conventions and everything is singular in the limit of zero coupling. On varying the coupling from repulsive to attractive, the two-boson state with the lowest possible center-of-mass energy goes from two bosons with slightly different real momenta k_1,k_2 for $c>0$ (repulsive) to identical momenta at $c=0$ to complex conjugate momenta $k\pm ic$ for $c<0$ (attractive). For c attractive, it is not possible for different real k_j to have the same $\tilde{I}_j$ (or I_j), but we can take complex conjugate momenta $k\pm ic$ to have the same quantum number. A similar analysis works for three or more bosons.

In the Bethe ansatz formulation of quantum sine-Gordon thermodynamics, one does not use the individual boson quantum numbers, but quantum numbers for the breathers, or j strings, which are treated quasifermionically. The content of our transformation in Sec. IV is that in the limit $g\to 0$ ($c\to 0^-$, attractive case), we can work in terms of the constituent bosons—the members of a string correspond to multiple occupation of a single boson quantum number. It is crucial to realize the further point that the bosonic entropy term we find is equivalent to assuming that in a small region of momentum space Δk all arrangements of bosons in available states are equivalent. This means we cannot distinguish between bosons in strings of different lengths, so our entropy expression is only good in the limit of zero binding energy for strings, that is, the zero coupling limit. This is what is different between the bosonizations for the repulsive and attractive cases—for the repulsive case, the bosonization is valid for any value of the coupling strength, in the sense that the thermodynamic analysis using the boson entropy term, etc., is exact. For the attractive case (or actually the weak-coupling limit of the sine-Gordon), the bosonization is only true in limit $c\to 0^-$ ($g\to 0$), and a thermodynamic analysis using the boson entropy term can only be approximately correct for a finite coupling strength. The classical sine-Gordon limit is limit $g\to 0$, and we conclude that finding quantum corrections (finite g) by these techniques will be difficult.

Finally, let us compare our analysis to the approach of gas phenomenology. If we adopt this approach, and simply assume that the breather ladder can somehow be replaced by a physical phonon, and that the phonons and solitons obey BA-type boundary condition equations with phase shifts θ_{pp}, θ_{ps}, and θ_{ss}, it is not difficult to follow a Yang-Yang–type procedure to get coupled fermionic and bosonic thermodynamic equations:

$$\ln\eta_p(\alpha)=\frac{m}{T}\cosh\alpha-\frac{1}{2\pi}\int_{-\infty}^{\infty}d\alpha'\theta'_{pp}(\alpha'-\alpha)\times\ln[1-\eta_p^{-1}(\alpha')]+\frac{2}{2\pi}\int_{-\infty}^{\infty}d\alpha'\theta'_{ps}(\alpha'-\alpha)\ln[1+\eta_s^{-1}(\alpha')]\,, \tag{5.12a}$$

$$\ln\eta_s(\alpha)=\frac{M}{T}\cosh\alpha-\frac{1}{2\pi}\int_{-\infty}^{\infty}d\alpha'\theta'_{ps}(\alpha'-\alpha)\times\ln[1-\eta_p^{-1}(\alpha')]\,.+\frac{2}{2\pi}\int_{-\infty}^{\infty}d\alpha'\theta'_{ss}(\alpha'-\alpha)\ln[1+\eta_s^{-1}(\alpha')]\,. \tag{5.12b}$$

It is interesting that the two equations we derived from the BA [Eqs. (4.16)] are very nearly of this form. We formally integrate the first integral in (5.12a) by parts and compare with (4.16) to identify the phase shifts

$$\theta_{pp}(\alpha)=-\frac{2\pi}{n}P\frac{1}{\sinh\alpha}\,,\qquad \theta_{ps}(\alpha)=2\tan^{-1}(\sinh\alpha)\,, \tag{5.13}$$

to go along with θ_{ss} given in (4.2).

VI. DISCUSSION

It is somewhat surprising that our method has given the classical sine-Gordon specific heat so accurately. After all, the classical system does have breather solutions, and even near the classical limit the ladder of allowed breather rest masses is not uniformly spaced over its whole range, as we have taken it to be. Yet our result is apparently accurate for temperatures of order the soliton mass, where we certainly expect the nonlinearities in the mass spectrum to be making an important contribution. That is to say, our basic integral equations give correct results in a temperature range where they cannot be physically interpreted in the obvious fashion—where there are nonvanishing densities of breathers with finite (phonon) binding energies, and the system cannot be physically understood in terms of soliton and phonon densities alone.

Let us review the approximations made in this paper, when we expect them to fail, and possible reasons why they don't. The basic approximation is that we have neglected the contribution of the phonon-phonon interaction to the breather energies (although these interactions were included in the phase shifts). That is to say, we have taken the breathers to represent bound states of phonons, but with the mass of the jth breather equal to jm (where $m\sim n^{-1}$ is the phonon mass). Thus we have dropped the $O(j^3/n^3)$ binding energy contribution. Similarly we have retained only the $O(n^{-1})$ terms in the breather-breather phase shifts, which gives a phase shift between a j breather and k breather equal to jk times an $O(n^{-1})$ phonon-phonon phase shift. These approximations—linearization of the breather mass spectrum and phase shifts—are consistent with interpreting the jth breather as j barely bound phonons, and they yield a pair of integral equations (4.16) for the soliton and anharmonic phonon densities which correctly reproduce the classical SG free energy to high order (4.20).

Let us focus on the anharmonic phonon contribution to the free energy. It seems at first sight very reasonable to include only the $O(n^{-1})$ term in the breather mass spectrum and phase shifts, since the phonon density is of order n in the classical limit. However, as one takes $n \to \infty$ at fixed $t = T/M$, the important breather contributions to the free energy should come from those breathers with $j \sim tn$. These breathers have a binding energy of order $j^3/n^3 \sim t^3$, and it is not obvious why we can compute the phonon free energy correct to t^6, say, with the breather binding energy neglected. The reason is not trivial—for example, if one computes the free energy using the nonuniform breather masses but (inconsistently) using the breather densities derived from our approximations, it turns out that there are nonvanishing contributions from the breather binding energies [i.e., from the $O(j^3/n^3)$ terms in the mass spectrum]. Of course, consistently including these binding energy terms in the masses and phase shifts need not affect the free energy to this order, because the distribution and hence entropy terms would adjust to minimize the free energy. (Once the binding energy terms are included, the bosonic entropy form is no longer valid, as discussed in Sec. V.)

Evidently, the approximations we have made—equally spaced breather mass spectrum and j-breather—k-breather phase shift proportional to jk, which lead to the bosonic expression for the entropy—are logically consistent, and correct in the classical limit at the bottom of the breather spectrum. Since the anharmonic phonon specific heat we calculate using these approximations is correct over a wide temperature range, the binding energy corrections must somehow cancel when retained in both the breather masses and phase shifts. It is interesting to note that in the sine-Gordon model, which is very similar to the repulsive boson gas, there are no phonon bound states so the phonon density gives the complete picture at all temperature. The classical sine-Gordon specific heat has been calculated and it is found that if one "analytically continues" the coupling to the classical sine-Gordon system one gets exactly the phonon series we have described above (4.20).[48] Thus we note that in this approach the formation of multiphonon bound states—breathers—does not affect the phonon specific-heat term.

The other approximation made in the above is dropping the $e^{-\pi/t}$ term in (4.15b). This is an upper end contribution from the sum over breather states, which becomes an integral in the classical limit. The π has no physical significance—it arises because we have taken an evenly spaced breather mass spectrum $M_j = jM\pi/n$ so the heaviest breather is assigned a mass πM rather than its actual value of $2M$. Hence the upper end contribution should really be of order $e^{-2/t}$. However, we have also taken phase shift values in deriving (4.15b) which are invalid at the upper end of the breather spectrum. In fact, our analysis is correct at least for the leading $e^{-2/t}$ term even with this upper end contribution neglected. The equations (4.16) (in which the $e^{-\pi/t}$ has been dropped) generate $e^{-2/t}$ terms arising from soliton-soliton and soliton-antisoliton interactions. Since the heavy breathers are very loosely bound soliton-antisoliton pairs, perhaps their contribution to the free energy is automatically included in the $e^{-2/t}$ terms generated, at least to some order. In our earlier publication,[39] we suggested that heavy breather terms might be one explanation for the discrepancy between our work and the transfer matrix results of Sasaki. More recently, however, Timonen *et al.*[41] have rechecked the transfer matrix method and find complete agreement with the Bethe ansatz results.

ACKNOWLEDGMENTS

We have greatly benefited from discussions with Kazumi Maki, who taught us how to do some integrals needed in the iteration procedure. We also wish to thank Kazuo Sasaki for helpful discussions of his work. We thank Robin Bullough and Jussi Timonen for sending us unpublished reports of their recent work, and for interesting discussions. Two of us (N.N.C. and M.F.) wish to thank J. R. Schrieffer for his hospitality at the Institute for Theoretical Physics, Santa Barbara, where this work was begun. The present paper was supported by the National Science Foundation under Grant No. DMR-84-04955.

APPENDIX A: BREATHER-SOLITON AND SOLITON-SOLITON PHASE SHIFTS

When $\mu = (1-n^{-1})\pi$, the soliton-breather and soliton-soliton phase shifts (2.7) can be written equivalently as

$$\theta_{js}(\alpha) = \tfrac{1}{2} f_{j,n-1}(\alpha), \quad j \le n-2 \tag{A1a}$$

$$\theta_{ss}(\alpha) = \tfrac{1}{4} f_{n-1,n-1}(\alpha) , \tag{A1b}$$

where f_{jk} is defined in (2.6). When $\mu = (1-n^{-1})\pi$, an $(n-1)$-string represents a soliton (s) and a hole in the Dirac sea is an antisoliton ($\bar{s}$). Thus the phase shift θ_{js} is, in BA language, the phase shift of a j string ($j \le n-2$) with either an $(n-1)$-string or a hole (these phase shifts are equal). Similarly, θ_{ss} is the phase shift between two holes or two $(n-1)$-strings or a hole and an $(n-1)$-string (all of which are equal); i.e., when $\mu - (1-n^{-1})\pi$, the soliton-antisoliton scattering is reflectionless and $\theta_{ss} = \theta_{s\bar{s}} = \theta_{\bar{s}\bar{s}}$.

Using (A1), Eqs. (2.3) can be written equivalently in the succinct form

$$(1+\delta_{j,n-1})\ln\eta_j = \frac{M_j}{T}\cosh\alpha + \frac{1}{2\pi}\sum_{k=1}^{n-1}\int_{-\infty}^{\infty} d\alpha' f'_{jk}(\alpha'-\alpha) \times \ln(1+\eta_k^{-1}) , \quad j = 1,2,\ldots,n-1 \tag{A2}$$

where the subscript $n-1$ replaces s in (2.3) and $M_{n-1} \equiv 2M$. It is important to note that M_{n-1} is *not* the mass of an $(n-1)$-string (which is actually M), and $f_{j,n-1}$ is *not* the phase shift with an $(n-1)$-string [these are given by (A.1)]. For $\mu = (1-n^{-1})\pi$, $\theta_{jk} = f_{jk}$ only for $j,k \le n-2$. The thermodynamic equations were presented in Refs. 38 and 39 in the form (A2), although in both papers the $1+\delta_{j,n-1}$ term was inadvertently omitted in print.

This paper is based entirely on the case $\mu=(1-n^{-1})\pi$ exactly, but it may be helpful to consider as an aside the limiting case $\mu=(1-n^{-1})\pi+\epsilon$ as $\epsilon\to 0$. In this limit, the lowest $n-2$ strings still represent DHN breathers, but the $(n-1)$-string also becomes a breather (of zero binding energy); and the holes in the Dirac sea combine with longer strings [not present in the case $\mu=(1-n^{-1})\pi$ exactly] to represent the unbound solitons and antisolitons.[37] Call the phase shifts in this limiting case θ^{ϵ}_{jk}, and define a function f^{ϵ}_{jk} of the form (2.6) but with the substitution

$$\theta^{\epsilon}(\alpha,j)=-i\ln\left[\frac{\sinh\alpha-i\sin\left[j\dfrac{\pi(\pi-\mu)}{2\mu}\right]}{\sinh\alpha+i\sin\left[j\dfrac{\pi(\pi-\mu}{2\mu}\right]}\right] \tag{A3}$$

in place of (2.6b), with $\mu=(1-n^{-1})\pi+\epsilon$. Then, for $j,k=1$ to $n-1$, $\theta^{\epsilon}_{jk}=f^{\epsilon}_{jk}$. Notice the inclusion of the $(n-1)$-string here—this is to be contrasted with the case $\mu=(1-n^{-1})\pi$ exactly, for which $\theta_{jk}=f_{jk}$ only for $j,k\le n-2$. As $\epsilon\to 0$, $\theta^{\epsilon}(\alpha,j)\to\theta(\alpha,j)$ except when $j=2n-2$, in which case $\theta^{\epsilon}(\alpha,2n-2)\to 2\pi H(\alpha)$ (step function) but $\theta(\alpha,2n-2)=0$. As a result, $f^{\epsilon}_{jk}=f_{jk}$, $j,k=1$ to $n-1$, except when $j=k=n-1$, for which $f^{\epsilon}_{n-1,n-1}(\alpha)=f_{n-1,n-1}(\alpha)+2\pi H(\alpha)$. The step-function piece is a consequence of the fact that, when $\mu=(1-n^{-1})\pi+\epsilon$, a new zero-binding-energy $s\bar{s}$ bound state is formed.

Since when $\mu=(1-n^{-1})\pi+\epsilon$ the $(n-1)$-string represents a barely bound $s\bar{s}$ pair, one should expect to find $\theta^{\epsilon}_{j,n-1}=\theta_{js}+\theta_{j\bar{s}}=2\theta_{js}$ $(j\le n-2)$; and in fact as $\epsilon\to 0$, $f^{\epsilon}_{j,n-1}=f_{j,n-1}$ and this is statement (A1a). Similarly, one might expect that $\theta^{\epsilon}_{n-1,n-1}$ is the sum of four phase shifts (ss $s\bar{s}$, $\bar{s}s$, and $\bar{s}\bar{s}$ and thus that $\theta^{\epsilon}_{n-1,n-1}=4\theta_{ss}$. However, because of the new $s\bar{s}$ bound state [compared with $\mu=(1-n^{-1})\pi$], the picture is a bit more complicated, and it turns out that

$$\begin{aligned}\theta^{\epsilon}_{n-1,n-1}(\alpha)=f^{\epsilon}_{n-1,n-1}(\alpha)&=f_{n-1,n-1}(\alpha)+2\pi H(\alpha)\\&=4\theta_{ss}(\alpha)+2\pi H(\alpha)\ ,\end{aligned} \tag{A4}$$

where θ_{ss} is the $\mu=(1-n^{-1})\pi$ hole-hole (or ss) phase shift (A1b). One can think of (A1b) by saying (loosely) that $f_{n-1,n-1}$ (no ϵ) represents the scattering between two barely bound $s\bar{s}$ pairs [i.e., two $\mu=(1-n^{-1})\pi+\epsilon$ $(n-1)$-strings] with the step-function terms neglected.

For completeness, here are the phase shifts between $(n-1)$-strings and holes, and just holes, when $\mu=(1-n^{-1})\pi+\epsilon$:

$$\begin{aligned}&\theta^{\epsilon}_{n-1,h}(\alpha)=2\theta_{ss}(\alpha)+2\pi H(\alpha)\ ,\\&\theta^{\epsilon}_{hh}(\epsilon)=\theta_{ss}(\alpha)\ .\end{aligned} \tag{A5}$$

In this limit the phase shifts involving longer strings (length $> n-1$) become step functions.[37]

APPENDIX B: LOW-TEMPERATURE EXPANSION OF THE FREE ENERGY

Here we summarize the solution of equations (4.16) for η_p and η_s and substitute the results into (4.18) to get the free energy. We expand in a double series in $e^{-1/t}$ and t, where $t=T/M$ is the reduced temperature. In the following, consider t small but fixed as $n\to\infty$. Our expansion follows the approach of Maki.[38]

The first two terms on the right-hand side of (4.16a) are of order $m/T=\pi/nt=O(n^{-1})$, so we are let to put

$$\ln\eta_p(\alpha)=(m/T)u(\alpha),\quad \eta_s^{-1}(\alpha)=(m/T)g(\alpha)\ , \tag{B1}$$

where we expect to find u and g of order unity. Then Eqs. (4.16) become

$$\begin{aligned}u(\alpha)=\cosh\alpha-\frac{t}{\pi}P\int_{-\infty}^{\infty}&\frac{d\alpha'}{\sinh(\alpha'-\alpha)}\frac{\partial}{\partial\alpha'}\\&\times\ln\{1-\exp[-(m/T)u(\alpha')]\}\\&+\frac{2}{\pi}\int_{-\infty}^{\infty}\frac{d\alpha'}{\cosh(\alpha'-\alpha)}g(\alpha')\ ,\end{aligned} \tag{B2a}$$

$$\begin{aligned}\ln g(\alpha)=-\frac{1}{t}\cosh\alpha+\frac{1}{\pi}\int_{-\infty}^{\infty}&\frac{d\alpha'}{\cosh(\alpha'-\alpha)}\ln u(\alpha')\\-\frac{1}{\pi t}\int_{-\infty}^{\infty}&d\alpha'\ln\left[\frac{\cosh(\alpha'-\alpha)+1}{\cosh(\alpha'-\alpha)-1}\right]g(\alpha')\ ,\end{aligned} \tag{B2b}$$

plus terms which vanish as $n\to\infty$. In the first integral in (B2a) the limit $m/T\to 0$ must be taken with some care, as we shall show. Separate the free energy (4.18) into direct contributions from the breather and soliton terms and then expand in powers of $e^{-1/t}$; then

$$\begin{aligned}F&=F^{(b)}+F^{(s)}=F_0+F_1+F_2+\cdots\ ,\\F^{(b)}&=\frac{mT}{2\pi}\int_{-\infty}^{\infty}d\alpha\cosh\alpha\ln\{1-\exp[-(m/T)u(\alpha)]\}\\&=F_0^{(b)}+F_1^{(b)}+F_2^{(b)}+\cdots\ ,\end{aligned} \tag{B3}$$

$$F^{(s)}=-\frac{mM}{\pi}\int_{-\infty}^{\infty}d\alpha\cosh\alpha\,g(\alpha)=F_1^{(s)}+F_2^{(s)}+\cdots\ ,$$

plus terms which vanish as $n\to\infty$. Our problem is to solve (B2) for u and g in order to calculate the free energy (B3).

Separate $u(\alpha)$ into pieces:

$$u(\alpha)=\cosh\alpha-h(\alpha)t+u_s(\alpha)\ , \tag{B4}$$

where

$$h(\alpha)=\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{d\alpha'}{\sinh(\alpha'-\alpha)}\frac{\partial}{\partial\alpha'}b(\alpha')\ , \tag{B5}$$

$$u_s(\alpha)=\frac{2}{\pi}\int_{-\infty}^{\infty}\frac{d\alpha'}{\cosh(\alpha'-\alpha)}g(\alpha')\ , \tag{B6}$$

and

$$b(\alpha)=\ln\{1-\exp[-(m/T)u(\alpha)]\}\ . \tag{B7}$$

Now expand in powers of $e^{-1/t}$ and t:

$$
\begin{aligned}
b(\alpha) &= \sum_{n=0}^{\infty} b_n(\alpha) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} b_{nm}(\alpha)t^m , \\
h(\alpha) &= \sum_{n=0}^{\infty} h_n(\alpha) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} h_{nm}(\alpha)t^m , \\
g(\alpha) &= \sum_{n=1}^{\infty} g_n(\alpha) = \sum_{n=1}^{\infty}\sum_{m=0}^{\infty} g_{nm}(\alpha)t^m , \\
u_s(\alpha) &= \sum_{n=1}^{\infty} u_n(\alpha) = \sum_{n=1}^{\infty}\sum_{m=0}^{\infty} u_{nm}(\alpha)t^m ,
\end{aligned}
\qquad \text{(B8)}
$$

where the lone or first subscript refers to the order in $e^{-1/t}$ and the second subscript to the power of t. Then an order-by-order comparison of the identity [B7) and (B4)]

$$
\begin{aligned}
b(\alpha) &= \ln\{1-\exp[-(m/T)\cosh\alpha]\} \\
&\quad + \ln\left[1-\frac{\exp[(m/T)(ht-u_s)]-1}{\exp[(m/T)\cosh\alpha]-1}\right] \\
&= \ln\{1-\exp[-(m/T)\cosh\alpha]\} \\
&\quad + \ln\left[1+\frac{u_s-ht}{\cosh\alpha}\right] + O(n^{-1})
\end{aligned}
\qquad \text{(B9)}
$$

leads to

$$
b_0(\alpha) = \ln\{1-\exp[-(m/T)\cosh\alpha]\} + \ln\left[1-\frac{h_0 t}{\cosh\alpha}\right] , \qquad \text{(B10a)}
$$

$$
b_1(\alpha) = \frac{u_1-h_1 t}{\cosh\alpha - h_0 t} , \qquad \text{(B10b)}
$$

$$
b_2(\alpha) = \frac{u_2-h_2 t}{\cosh\alpha - h_0 t} - \tfrac{1}{2}(b_1)^2 , \qquad \text{(B10c)}
$$

$$\vdots$$

Equating terms of equal order in (B5) gives

$$
h_{nm}(\alpha) = \frac{P}{\pi}\int_{-\infty}^{\infty} \frac{d\alpha'}{\sinh(\alpha'-\alpha)} \frac{\partial}{\partial\alpha'} b_{nm}(\alpha') . \qquad \text{(B11)}
$$

Finally, from (B2b), (B4), and (B8) we find that

$$
\begin{aligned}
g(\alpha) &= (1+\cosh\alpha)\exp[-(1/t)\cosh\alpha] \\
&\quad \times \exp(I_0+I_1+I_2+\dots) ,
\end{aligned}
\qquad \text{(B12)}
$$

where

$$
I_0(\alpha) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{d\alpha'}{\cosh(\alpha'-\alpha)} \ln\left[1-\frac{h_0 t}{\cosh\alpha'}\right] , \qquad \text{(B13a)}
$$

$$
\begin{aligned}
I_n(\alpha) &= \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{d\alpha'}{\cosh(\alpha'-\alpha)} b_n(\alpha') \\
&\quad - \frac{1}{\pi t}\int_{-\infty}^{\infty} d\alpha' \ln\left[\frac{\cosh(\alpha'-\alpha)+1}{\cosh(\alpha'-\alpha)-1}\right] g_n(\alpha'),
\end{aligned}
\qquad n>0 \quad \text{(B13b)}
$$

and where we have used the result

$$
\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{d\alpha'}{\cosh(\alpha'-\alpha)} \ln(\cosh\alpha') = \ln(1+\cosh\alpha) . \qquad \text{(B14)}
$$

For each value of n (i.e., order in $e^{-1/t}$), Eqs. (B10) and (B11) are used to compute h_{nm} and b_{nm} alternately; then with (B12) and (B6) these give g_{n+1} and u_{n+1}. From (B3), (B7), and (B8), the order $e^{-n/t}$ (so-called n-soliton) contributions to F can be written as

$$
F_n^{(b)} = \frac{mT}{2\pi}\int_{-\infty}^{\infty} d\alpha \cosh\alpha\, b_n(\alpha), \quad n\ge 0 \qquad \text{(B15a)}
$$

$$
F_n^{(s)} = -\frac{mM}{\pi}\int_{-\infty}^{\infty} d\alpha \cosh\alpha\, g_n(\alpha), \quad n\ge 1 . \qquad \text{(B15b)}
$$

In principle, this iterative procedure can be used to give F to all orders.

1. Phonon contribution ($n=0$)

The $n=0$ or phonon contribution to the free energy is, from (B15a) and (B8),

$$
F_0 = F_0^{(b)} = \frac{mM}{2\pi}\int_{-\infty}^{\infty} d\alpha \cosh\alpha \sum_{m=0}^{\infty} b_{0m}(\alpha)t^{m+1} . \qquad \text{(B16)}
$$

Equation (B10a) gives

$$
b_{00} = \ln\{1-\exp[-(m/T)\cosh\alpha]\} , \qquad \text{(B17a)}
$$

$$
b_{01} = -h_{00}\operatorname{sech}\alpha , \qquad \text{(B17b)}
$$

$$
b_{02} = -h_{01}\operatorname{sech}\alpha - \tfrac{1}{2}(b_{01})^2 , \qquad \text{(B17c)}
$$

$$\vdots$$

The alternating solution of (B11) and (B17) hinges on the evaluation of h_{00} as $m/T\to 0$. From (B11) and (B17a) it is easy to show that

$$
h_{00}(\alpha) \approx \operatorname{sech}\alpha, \quad |\alpha| \ll \ln(T/m) \qquad \text{(B18)}
$$

plus finite corrections for α of order $\ln(T/m)$. Nearly everywhere h_{00} is used, the large-α corrections are suppressed by another factor [e.g., h_{00} is divided by $\cosh\alpha$ in (B17b)] and hence vanish as $n\to\infty$. The exception is the $m=1$ term in the free energy (B16), which needs special attention (see Appendix C).

Using h_{00} from (B18), now (B11) and (B17) can be used to compute b_{om} and h_{om} alternately. We find

$$
\begin{aligned}
b_{01} &= -\operatorname{sech}^2\alpha , \\
h_{01} &= 2\operatorname{sech}^3\alpha - \operatorname{sech}\alpha , \\
b_{02} &= -\tfrac{5}{2}\operatorname{sech}^4\alpha + \operatorname{sech}^2\alpha , \\
h_{02} &= 10\operatorname{sech}^5\alpha - 7\operatorname{sech}^3\alpha - \tfrac{1}{4}\operatorname{sech}\alpha , \\
&\ \ \vdots
\end{aligned}
\qquad \text{(B19)}
$$

Substituting b_{0m} from (B19) and (B17a) into (B16) (expect for the $m=1$ term, which is computed in Appendix C), the phonon contribution to the free energy becomes

$$
\begin{aligned}
F_0 &= F_{\text{non}} - mM(\tfrac{1}{4}t^2 + \tfrac{1}{8}t^3 + \tfrac{3}{16}t^4 \\
&\quad + \tfrac{53}{128}t^5 + \tfrac{297}{256}t^6 + \cdots)
\end{aligned}
\qquad \text{(B20)}
$$

where

$$F_{\text{non}} = \frac{mT}{2\pi} \int_{-\infty}^{\infty} d\alpha \cosh\alpha \ln\{1 - \exp[-(m/T)\cosh\alpha]\} \tag{B21}$$

is the noninteracting phonon free energy found in Sec. III.

2. One-soliton contribution ($n = 1$)

The order $e^{-1/t}$ (i.e., $n = 1$) contribution to F, the so-called one-soliton contribution, consists of two pieces: $F_1^{(s)}$ directly from solitons, and $F_1^{(b)}$ from breathers. First we will compute $F_1^{(s)}$ (B15b). Expanding (B13a) in powers of t and using h_{0m} from (B18) and (B19), we find from (B12) that

$$g_1(\alpha) = (1+\cosh\alpha) e^{(-1/t)\cosh\alpha} e^{I_0}$$
$$= 2e^{(-1/t)\cosh\alpha} \left[\cosh^2\frac{\alpha}{2} - \frac{t}{2} - \frac{t^2}{16} \times \left[3\,\text{sech}^2\frac{\alpha}{2} + 2 \right] + \cdots \right]. \tag{B22}$$

$F_1^{(s)}$ in Eq. (B15b) can be evaluated using (B22) and the change of variables $2\sinh(\alpha/2) = t^{1/2}x$ to give

$$F_1^{(s)} = -2mM \left[\frac{2t}{\pi} \right]^{1/2} e^{-1/t} (1 + \tfrac{1}{8}t - \tfrac{43}{128}t^2 - \tfrac{601}{1024}t^3 - \tfrac{42525}{32768}t^4 + \cdots). \tag{B23}$$

Similarly, from (B6) and (B22), we can calculate

$$u_1(\alpha) = A\,\text{sech}\alpha[1 - t(\text{sech}^2\alpha - \tfrac{1}{8}) + t^2(3\,\text{sech}^4\alpha - \tfrac{17}{8}\text{sech}^2\alpha - \tfrac{43}{128}) + \cdots], \tag{B24}$$

where $A = 4(2t/\pi)^{1/2} e^{-1/t}$. As in the $n = 0$ case, now (B10b) and (B11) are used to compute b_{1m} and h_{1m} alternately:

$$\begin{aligned}
b_{10} &= A\,\text{sech}^2\alpha , \\
h_{10} &= A(-2\,\text{sech}^3\alpha + \text{sech}\alpha) , \\
b_{11} &= A(2\,\text{sech}^4\alpha - \tfrac{7}{8}\text{sech}^2\alpha) , \\
h_{11} &= A(-8\,\text{sech}^5\alpha + \tfrac{23}{4}\text{sech}^3\alpha + \tfrac{1}{8}\text{sech}\alpha) , \\
&\vdots
\end{aligned} \tag{B25}$$

The $n = 1$ breather contribution is computed by putting (B25) into (B15a):

$$F_1^{(b)} = 2mM \left[\frac{2t}{\pi} \right]^{1/2} e^{-1/t} (t + \tfrac{1}{8}t^2 + \tfrac{37}{128}t^3 + \tfrac{1015}{1024}t^4 + \cdots), \tag{B26}$$

and the total one-soliton free energy is the sum of (B23) and (B26):

$$F_1 = F_1^{(s)} + F_1^{(b)}$$
$$= -2mM \left[\frac{2t}{\pi} \right]^{1/2} e^{-1/t} \times (1 - \tfrac{7}{8}t - \tfrac{59}{128}t^2 - \tfrac{897}{1024}t^3 - \tfrac{75005}{32768}t^4 + \cdots). \tag{B27}$$

3. Two-soliton contribution ($n = 2$)

The order $e^{-2/t}$, or two-soliton, contribution is similarly the sum of a soliton and a breather contribution (B3), and we first compute the former [Eq. (B15b)]. From (B12) and (B22),

$$g_2(\alpha) = g_1(\alpha) I_1(\alpha). \tag{B28}$$

Using (B13b) we put

$$I_1 = I_{1b} + I_{1s}, \tag{B29}$$

where

$$I_{1b} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\alpha'}{\cosh(\alpha' - \alpha)} b_1(\alpha'), \tag{B30}$$

$$I_{1s} = -\frac{1}{\pi t} \int_{-\infty}^{\infty} d\alpha' \ln \left[\frac{\cosh(\alpha'-\alpha)+1}{\cosh(\alpha'-\alpha)-1} \right] g_1(\alpha'), \tag{B31}$$

and b_1 and g_1 are given by (B25) and (B22), respectively. We find

$$I_{1b} = A \left[\tfrac{1}{2}\,\text{sech}^2\frac{\alpha}{2} + t\left[\tfrac{1}{4}\,\text{sech}^4\frac{\alpha}{2} + \tfrac{1}{16}\,\text{sech}^2\frac{\alpha}{2} \right] + \cdots \right]. \tag{B32}$$

To compute I_{1s}, change variables to $x = (2t)^{-1/2}\alpha$ and expand the integrand of (B31) in powers of t; the result is

$$I_{1s} = -At^{-1}\{ [\tfrac{1}{2}\ln(2/t) - K_0(x)] + t[\tfrac{1}{12} - \tfrac{3}{16}\ln(2/t) + \frac{x^2}{6} + \tfrac{1}{6}K_4(x) - \tfrac{1}{2}K_2(x) + \tfrac{1}{2}K_0(x)] + \cdots \}, \tag{B33}$$

where

$$K_{2n}(x) \equiv \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dt\, t^{2n} e^{-t^2} \ln|t - x| \tag{B34}$$

and where we have used

$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dt\, t^{2n} e^{-t^2} = \frac{(2n-1)!!}{2^n}. \tag{B35}$$

We next rewrite K_{2n} in a simpler form. Divide the integral in (B34) into two pieces which define two functions h_1 and h_2:

$$\int_{-\infty}^{\infty} = \int_{-\infty}^{x} + \int_{x}^{\infty} = h_1(x) + h_2(x). \tag{B36}$$

By putting

$$h_i(x) = h_i(0) + \int_0^x h_i'(y)dy,$$

we find

$$K_{2n}(x)=\frac{2}{\sqrt{\pi}}\int_0^\infty dt\, t^{2n}e^{-t^2}e^{-t^2}\ln t + \frac{1}{\sqrt{\pi}}\int_0^x dy\, P\int_{-\infty}^{\infty} dt\frac{t^{2n}}{y-t}e^{-t^2} . \quad (B37)$$

Two integral representations of the error function give

$$P\int_{-\infty}^{\infty} dt\frac{e^{-t^2}}{y-t}=2\sqrt{\pi}e^{-y^2}\int_0^y e^{t^2}dt , \quad (B38)$$

which, together with (B37), yields

$$K_0(x)=-\tfrac{1}{2}\ln(4\gamma)+2F_0(x) ,$$
$$K_2(x)=-\tfrac{1}{4}\ln(4\gamma)+\tfrac{1}{2}-\tfrac{1}{2}x^2+2F_2(x) , \quad (B39)$$
$$K_4(x)=-\tfrac{3}{8}\ln(4\gamma)+1-\tfrac{1}{4}(x^2+x^4)+2F_4(x) ,$$
$$\vdots$$

where

$$F_{2n}(x)=\int_0^x dy\, e^{-y^2}y^{2n}\int_0^y dt\, e^{t^2} \quad (B40)$$

and Euler's constant $C=\ln\gamma=0.577\,215\,66\ldots$. In terms of F's, (B33) becomes

$$I_{1s}=-At^{-1}\left\{\left[\frac{1}{2}\ln\left[\frac{8\gamma}{t}\right]-2F_0(x)\right] + t\left[-\tfrac{3}{16}\ln\left[\frac{8\gamma}{t}\right]+\frac{3}{8}x^2-\frac{x^4}{24}+F_0(x) - F_2(x)+\tfrac{1}{3}F_4(x)\right]+\cdots\right\} . \quad (B41)$$

The direct-soliton contribution $F_2^{(s)}$ is found by inserting g_2 from (B28) into (B15b) [using (B22), (B29), (B32), and (B41)], changing variables in (B15b) to $x=(2t)^{-1/2}\alpha$, and expanding in t, we find

$$F_2^{(s)}=\frac{16}{\pi}mMe^{-2/t}\left\{\left[\frac{1}{2}\ln\left[\frac{8\gamma}{t}\right]-2G(0,0)\right]+t\left[-\frac{11}{32}-\frac{1}{8}\ln\left[\frac{8\gamma}{t}\right]+2G(0,0)-G(0,2) + \frac{1}{3}G(0,4)-3G(2,0)+\frac{1}{3}G(4,0)\right]+\cdots\right\} , \quad (B42)$$

where

$$G(n,m)\equiv\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} dx\, x^n e^{-x^2}F_m(x) . \quad (B43)$$

By changing variables in $F_{2n}(x)$ (B40) to $\xi=x^{-1}y$ and $\sigma=y^{-1}t$ and performing the x integral in (B43) first, it is a simple although tedious matter to compute $G(n,m)$. This procedure gives

$$F_2^{(s)}=\frac{8}{\pi}mMe^{-2/t}\left\{\ln\left[\frac{4\gamma}{t}\right]-t\left[\frac{1}{4}\ln\left[\frac{4\gamma}{t}\right]+\frac{5}{4}\right]-t^2\left[\frac{21}{32}\ln\left[\frac{4\gamma}{t}\right]+\frac{5}{16}\right]+\cdots\right\} . \quad (B44)$$

Finally we turn to the computation of the breather term $F_2^{(b)}$. First u_2 is computed by inserting g_2 into (B6) to give an integral similar in structure to $F_2^{(s)}$ above, which yields:

$$u_2(\alpha)=-\frac{16}{\pi}e^{-2/t}\left[\ln\left[\frac{4\gamma}{t}\right]\operatorname{sech}\alpha-t\left\{\frac{1}{4}\left[\ln\left[\frac{4\gamma}{t}\right]+5\right]\operatorname{sech}\alpha+\left[\ln\left[\frac{4\gamma}{t}\right]-1\right]\operatorname{sech}^3\alpha\right\}+\cdots\right] . \quad (B45)$$

Then (B10c) and (B11) can be solved for b_{2m} and h_{2m} alternately:

$$b_{20}=-\frac{16}{\pi}e^{-2/t}\ln\left[\frac{4\gamma}{t}\right]\operatorname{sech}^2\alpha ,$$
$$h_{20}=\frac{16}{\pi}e^{-2/t}\ln\left[\frac{4\gamma}{t}\right](2\operatorname{sech}^3\alpha-\operatorname{sech}\alpha) , \quad (B46)$$
$$b_{21}=-\frac{16}{\pi}e^{-2/t}\left[\ln\left[\frac{4\gamma}{t}\right]+1\right] \times(2\operatorname{sech}^4\alpha-\tfrac{5}{4}\operatorname{sech}^2\alpha) ,$$

and inserting the b_{2m} into (B15a) gives

$$F_2^{(b)}=\frac{8}{\pi}mMe^{-2/t}\left\{-t\ln\left[\frac{4\gamma}{t}\right] + \frac{1}{4}t^2\left[\ln\left[\frac{4\gamma}{t}\right]+1\right]+\cdots\right\} . \quad (B47)$$

The sum of (B44) and (B47) is the total two-soliton ($n=2$) contribution to F:

$$F_2=\frac{8}{\pi}mMe^{-2/t}\left\{\ln\left[\frac{4\gamma}{t}\right]-\frac{5}{4}t\left[\ln\left[\frac{4\gamma}{t}\right]+1\right] -t^2\left[\frac{13}{32}\ln\left[\frac{4\gamma}{t}\right]+\frac{1}{16}\right]+\cdots\right\} . \quad (B48)$$

APPENDIX C: COMPUTATION OF $F_{01}^{(b)}$

In the computation of $F_{01}^{(b)}$ (the lowest nonlinear phonon contribution to the free energy), the limit $m/T \to 0$ must be taken carefully. The expression (B17b) must be replaced by the exact value

$$b_{01}(\alpha) = -\frac{\epsilon h_{00}(\alpha)}{e^{\epsilon\cosh\alpha}-1}, \tag{C1}$$

where $\epsilon = m/T$; then from (B16), (C1), (B11), and (B17a),

$$F_{01}^{(b)} = -\frac{mMt^2}{2\pi} I, \tag{C2}$$

where

$$I = \lim_{\epsilon\to 0} \int_{-\infty}^{\infty} d\alpha \frac{\epsilon\cosh\alpha}{e^{\epsilon\cosh\alpha}-1} h_{00}(\alpha), \tag{C3}$$

$$h_{00}(\alpha) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{d\alpha'}{\sinh(\alpha'-\alpha)} \frac{\epsilon\sinh\alpha'}{e^{\epsilon\cosh\alpha'}-1}. \tag{C4}$$

By Fourier transformation (C3) becomes

$$I = \lim_{\epsilon\to 0} 4\pi \int_{-\infty}^{\infty} dx \tanh\left[\frac{\pi x}{2}\right] f(x) g(x), \tag{C5}$$

where

$$f(x) = \frac{1}{\pi} \int_0^{\infty} d\alpha \cos(\alpha x) \frac{\epsilon\cosh\alpha}{e^{\epsilon\cosh\alpha}-1}, \tag{C6a}$$

$$g(x) = \frac{1}{\pi} \int_0^{\infty} d\alpha \sin(\alpha x) \frac{\epsilon\sinh\alpha}{e^{\epsilon\cosh\alpha}-1}. \tag{C6b}$$

In the limit $\epsilon \to 0$, use of

$$\frac{\epsilon\cosh\alpha}{e^{\epsilon\cosh\alpha}-1} \approx \frac{1}{1+\frac{1}{2}\epsilon\cosh\alpha} \tag{C7}$$

in (C6) accurately gives I; this yields

$$f(x) \approx \coth\beta \frac{\sin\beta x}{\sinh\pi x}, \tag{C8a}$$

$$g(x) \approx \frac{1}{2} \frac{1}{\sinh\frac{\pi x}{2}} - \frac{\cos\beta x}{\sinh\pi x}, \tag{C8b}$$

where $\cosh\beta = 2/\epsilon$. Then inserting (C8) into (C5) gives

$$I = \lim_{\beta\to\infty} \left[\left[\pi - \frac{2\beta}{\sinh\beta} \right] + \left[-\frac{\pi}{2} + \frac{2}{\pi} \frac{\beta^2}{\sinh^2\beta} \right] \right] = \frac{\pi}{2} \tag{C9}$$

so that (C2) becomes

$$F_{01}^{(b)} = -\tfrac{1}{4} mMt^2. \tag{C10}$$

[1] J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B **11**, 3535 (1975).
[2] A. C. Scott, F. Y. F. Chu, D. W. McLaughlin, Proc. IEEE **61**, 1443 (1973).
[3] R. F. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. D **11**, 3424 (1975).
[4] R. Rajaraman, *Solitons and Instantons* (North-Holland, Amsterdam, 1982).
[5] K. Maki, in *Progress in Low Temperature Physics*, edited by D. F. Brewer (North-Holland, Amsterdam, 1982), Vol. VIII, Chap. 1.
[6] K. M. Leung, D. W. Hone, D. L. Mills, P. S. Riseborough, and S. E. Trullinger, Phys. Rev. B **21**, 4017 (1980).
[7] H. J. Mikeska, J. Phys. C **13**, 2913 (1980).
[8] H. J. Mikeska, J. Appl. Phys. **52**, 1950 (1981).
[9] K. Maki, Phys. Rev. B **24**, 3991 (1981).
[10] F. Borsa, Phys. Rev. B **25**, 3430 (1982).
[11] F. Borsa, M. G. Pini, A. Rettori, and V. Tognetti, Phys. Rev. B **28**, 5173 (1983).
[12] M. D. Johnson and N. F. Wright, Phys. Rev. B **32**, 5798 (1985).
[13] N. Gupta and B. Sutherland, Phys. Rev. A **14**, 1790 (1976).
[14] T. Schneider and E. Stoll, Phys. Rev. B **22**, 5317 (1980).
[15] K. Sasaki, Prog. Theor. Phys. **68**, 411 (1982).
[16] K. Sasaki and T. Tsuzuki, J. Magn. Magn. Mater. **31-34**, 1283 (1983).
[17] K. Sasaki, Prog. Theor. Phys. **71**, 1169 (1984).
[18] J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **22**, 477 (1980).
[19] N. Theodorakopoulos, Phys. Rev. B **30**, 4071 (1984).
[20] H. Takayama and M. Ishikawa, Prog. Theor. Phys. **74**, 479 (1984).
[21] K. Sasaki, Phys. Rev. B **33**, 2214 (1986).
[22] K. Maki and H. Takayama, Phys. Rev. B **20**, 3223 (1979).
[23] K. Maki and H. Takayama, Phys. Rev. B **20**, 5002 (1979).
[24] H. Takayama and K. Maki, Phys. Rev. B **21**, 4558 (1980).
[25] H. Takayama and K. Wada, J. Phys. Soc. Jpn. **50**, 3549 (1981).
[26] T. Miyashita and K. Maki, Phys. Rev. B **28**, 6733 (1983).
[27] T. Miyashita and K. Maki, Phys. Rev. B **31**, 1836 (1985).
[28] H. Bergknoff and H. B. Thacker, Phys. Rev. D **19**, 3666 (1979).
[29] V. E. Korepin, Teor. Mat. Fiz. **41**, 169 (1979) [Theor. Math. Phys. (USSR) **41**, 953 (1979)].
[30] H. B. Thacker, Rev. Mod. Phys. **53**, 253 (1981).
[31] M. Fowler and X. Zotos, Phys. Rev. B **24**, 2634 (1981).
[32] M. Fowler and X. Zotos, Phys. Rev. B **25**, 5806 (1982).
[33] X. Zotos and M. Fowler, Phys. Rev. B **26**, 1430 (1982).
[34] M. Fowler, Phys. Rev. B **26**, 2514 (1982).
[35] M. Imada, K. Hida, and M. Ishikawa, J. Phys. C **16**, 35 (1983).
[36] K. Hida, M. Imada, and M. Ishikawa, J. Phys. C **16**, 4945 (1983).
[37] M. D. Johnson, and M. Fowler, Phys. Rev. B **31**, 536 (1985).
[38] K. Maki, Phys. Rev. B **32**, 3075 (1985).
[39] N. N. Chen, M. D. Johnson, and M. Fowler, Phys. Rev. Lett. **56**, 904 (1986); **56**, 1427 (1986).
[40] R. K. Bullough, D. J. Pilling, and J. Timonen, in *Nonlinear Phenomena in Physics*, edited by F. Claro (Springer, Berlin, 1985), p. 103. These authors present their version of bosonization in *Coherence, Cooperation and Fluctuations*, edited by F. Haake, L. M. Narducci and D. F. Walls (Cambridge

University Press, Cambridge, 1986); *Dynamical Problems in Soliton Systems,* edited by S. Takeno (Springer-Verlag, Heidelberg, 1985). p. 105; Physica **18D**, 368 (1986).
[41]J. Timonen, M. Stirland, D. J. Pilling, Yi Cheng, and R. K. Bullough, Phys. Rev. Lett. **56**, 2233 (1986).
[42]E. H. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963).
[43]E. H. Lieb, Phys. Rev. **130**, 1616 (1963).
[44]C. N. Yang and C. P. Yang, J. Math. Phys. **10**, 1115 (1969).
[45]M. Wadati, J. Phys. Soc. Jpn. **54**, 3727 (1985).
[46]S. Coleman, Phys. Rev. D **11**, 2088 (1975).
[47]J. des Cloizeaux and M. Gaudin, J. Math. Phys. **7**, 1384 (1966).
[48]R. K. Bullough, D. J. Pilling, and J. Timonen (unpublished).