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Bethe-ansatz quantum sine-Gordon thermodynamics. The specific heat

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The Bethe-ansatz equations for the thermodynamic properties of the quantum sine-Gordon systems are derived in the zero-charge-sector attractive case. For rational values of the coupling parameter μ/π these reduce to a finite set, solved here numerically for $\mu=[(n-1)/n]\pi$, for several values of n, to give the specific heat as a function of temperature. The "soliton" contribution peaks at $\simeq$0.4 soliton masses for $\mu=\frac{4}{5}\pi$, shifting downward for higher μ. A detailed analysis of the sine-Gordon limit of the *XYZ* spin chain is presented, and a non-Lorentz-invariant feature of that limit is noted.

I. INTRODUCTION

This is the second paper in a series[1] developing the Bethe-ansatz approach to the finite-temperature properties of the quantum sine-Gordon (SG) system, using the methods and formalism developed by Takahashi and Suzuki[2] (TS) and Takahashi[3] for analyzing the thermodynamics of the *XXZ* and *XYZ* spin chains.

The first thermodynamic analysis of a Bethe-ansatz (BA) system was that given by Yang and Yang[4] for a one-dimensional Bose gas with repulsive δ-function interaction between particles. These authors assumed that the finite-temperature system could be represented by a density of excitations in $\vec{k}$ space (k being the particle momentum label appearing in the BA wave function) with an entropy arising from the number of microscopic arrangements corresponding to the given macroscopic density distribution. They found two coupled integral equations for the densities of filled and empty states in $\vec{k}$ space, one given by the usual BA boundary condition for the microscopic k variables, one by functional minimization of the free energy with respect to the density function.

This scheme was extended to the *XXZ* and *XYZ* models by Takahashi and Suzuki.[2] Although the basic idea is the same as for the Bose gas, the bookkeeping required becomes formidable, because there are many allowed bound states of magnons. A bound state of n magnons corresponds to a string of n complex rapidities, as discussed in detail in I. (We use the term "rapidity" to denote that parametrization of quasimomentum k for which phase shifts assume a difference form.) At finite temperatures, it is necessary to introduce density functions for filled and empty states for all allowed string lengths n—that is, for those n corresponding to normalizable wave functions, in general an infinite set. Which particular string lengths correspond to normalizable states depends on the coupling parameter μ (see I). The *XXZ*, *XYZ*, and SG models can all be parametrized in terms of the same variable μ in such a way that for a given value of μ they have the same sequence of allowed bound states. Consequently, the formalism set up by TS for the *XXZ* and *XYZ* models is easily adapted to the SG case. Furthermore, for certain values of μ, and in particular for $\mu=[(n-1)/n]\pi$ (n integer), the equations for string densities beyond a certain string length have a rather simple form. TS assumed that these equations could be reformulated in terms of a finite number of strings. In Sec. II, we give a detailed analysis of the bound states for these special values of μ, and show that the assumption of TS is correct. Hence the thermodynamic properties of the system are determined by a finite set of coupled integral equations. We have solved these equations numerically in the SG model for several values of n, we present the results for $n=5$ and 10.

The first step in solving the SG thermodynamic equations is to reformulate them in terms of dressed excitations. In terms of bare particles, the integrals appearing in the BA boundary condition equations extend over the whole Fermi sea, with the usual divergence problems. Transforming to dressed particles, the divergences are absorbed into the zero-temperature mass renormalizations, and the transformed integrals extend only to those parts of the Fermi sea thermally excited at a given temperature. This type of transformation is useful for analyzing the low-temperature properties of any BA system, and was used by Takahashi to examine the low-temperature specific heat of the *XXZ* and *XYZ* chains. For the SG case, the transformation is essential, because the mass renormalization is infinite. The new equations are of the familiar BA type, but with the fully renormalized (zero-temperature) dispersion curves and phase shifts appearing.

Formally, then, our scheme is very close to the phenomenological model of Currie, Krumhansl, Bishop, and Trullinger.[5] For the special values of coupling $\mu=[(n-1)/n]\pi$, the finite number of allowed strings which appear in the thermodynamic equations correspond exactly to the Dashen-Hasslacher-Neveu[6] (DHN) excitations. The equations give the densities of the DHN excitations as functions of temperature, taking into account their mutual phase shifting. However, in our approach it is clear when this scheme is valid—and how it can be extended, as we discuss later. It is only correct when the coupling parameter μ has a special value $[(n-1)/n]\pi$, n an integer. (In earlier work, Takahashi[7] assumed a scheme analogous to this was true for general coupling in the *XXZ* spin chain. It was pointed out by Johnson, McCoy, and Lai[8] that this gave incorrect results in the low orders of high-temperature perturbation theory. Their error estimate goes to zero for the special values of μ.)

It is evident from the above discussion why the analysis of Currie *et al.*[5] gives the right results in the classical limit. The semiclassical regime corresponds to μ slightly less than π. The special values $\mu=[(n-1)/n]\pi$, for which only DHN strings are needed, have a point of accumulation at the classical limit. Invoking Araki's theorem,[9] that the free energy at finite temperature is an analytic function of coupling, we deduce that neglect of the non-DHN strings is an increasingly good approximation as the classical limit is approached.

In the quantum regime, the special values $\mu=[(n-1)/n]\pi$ are further apart, and neglect of non-DHN strings is no longer valid. However, other rational values such as $\mu=[(n-2)/2]\pi$ give only slightly more complicated finite sets of integral equations which can be solved to find the thermodynamics. Again, interpolation between these values will give a reliable finite-temperature picture, from Araki's theorem. The essential difference between the special values $\mu=[(n-1)/n]\pi$ and more general rational μ/π is that in the latter case the basic set of excitations in the equations is wider than the DHN set.

Our results are presented in Sec. III. At very low temperatures, we find the exponential rise in specific heat is determined by the soliton mass for $\mu<\frac{3}{4}\pi$, and the phonon mass for $\mu>\frac{3}{4}\pi$, as discussed previously.[10] (We are working in the zero charge subspace—there is no finite soliton density at zero temperature in this paper.) At very high temperatures, the specific heat tends to that of the free-phonon gas (the SG coupling becomes irrelevant). After subtracting the free-phonon specific heat, we find a peak in the "soliton" specific heat at $\simeq$0.4 soliton masses for $\mu=\frac{4}{5}\pi$. For $\mu=\frac{9}{10}\pi$, the peak is smaller and at a lower temperature. Presumably, as $\mu\rightarrow\pi$ the position of the peak tends to some finite fraction of the soliton mass. For a particular classical SG chain, Schneider and Stoll[11] find the peak at about a quarter of a soliton mass, and the present results are not inconsistent with that limit. We emphasize that the term soliton specific heat as used here means simply the total specific heat minus that corresponding to the free-phonon gas. We do not know how to separate the contributions to specific heat from solitons, phonons, and breathers, or even if such a separation can be defined. In fact, our results indicate that as the classical limit is approached the deviation of the total specific heat from that of the free-phonon gas becomes smaller and smaller. It should be noted that our (lattice) energy cutoff is far above the soliton mass, so that even at high temperatures the phonon specific heat is linear in temperature. This nonclassical feature of our "classical limit" is of course in contrast with true classical lattice models,[11,12] where the phonon specific heat is constant. The point is, of course, that the limit $h\rightarrow0$ does not commute with the limit $\Lambda\rightarrow\infty$ where Λ is the momentum space cutoff needed for a finite specific heat.

Only the attractive sine-Gordon system is considered in this paper. For the strongly repulsive case ($\mu<\pi/3$), Korepin[13] has shown that the ground-state structure changes, and the continuum sine-Gordon model no longer coincides with the spin chain limit. We believe that the techniques described in this paper could be extended to the repulsive case.

Finally, we note that the sine-Gordon system defined as a limit of an *XYZ* chain has non-Lorentz invariant dressing, discussed in detail in Sec. II. However, our analysis is carried out entirely in terms of dressed excitations, so this difficulty does not appear, and in fact the dressed equations could have been derived from a continuum sine-Gordon model.

II. FORMALISM FOR SG THERMODYNAMICS

A. Preliminaries

The formal structure of a Yang and Yang[4] thermodynamic analysis of the SG system is, as already discussed, essentially equivalent to that of TS (Ref. 2) for the *XXZ* and *XYZ* models. For convenience, we have summarized their results in Appendix A.

One obvious way to arrive at the equations describing SG thermodynamics is to take the TS equations for the *XYZ* chain to the continuum limit shown by Luther[14] and Bergknoff and Thacker[15] to be equivalent to the SG system. The details of this limiting process in the TS formalism are given in Appendix B. Actually, it is not really necessary to follow this route—one could instead begin with the continuum SG Hamiltonian, defined (following Korepin[16]) with a cutoff Λ in momentum space. The thermodynamic equations we use—those for the dressed excitations—are the same in both approaches.

A delicate point in the spin chain continuum limit, which seems not to have been previously noted, is that the limiting velocity (velocity of light) is different for bare and dressed particles. The simplest way to see that this must be true is to consider the massless Thirring model, corresponding to the continuum limit of the *XXZ* chain. The bare excitation dispersion curve is[15]

$$\epsilon_{XXZ}^{(0)} = (J_z \sin\mu) ka \quad , \tag{2.1}$$

where a is the lattice spacing, and the dressed excitations have energy[17]

$$\epsilon_{XXZ} = [J_z(\pi/2\mu) \sin\mu] ka \quad . \tag{2.2}$$

The continuum limit is given by $a \to 0$, $J_z \to \infty$ so that the energies remain finite for finite k. We shall take

$$J_z = 2\mu/\pi a \sin\mu \tag{2.3}$$

giving unit velocity for the dressed excitations, but velocity $2\mu/\pi$ for the bare excitations. This same ratio of (limiting) velocities arises in the massive Thirring model at large momenta. The details are presented in Appendix B.

The origin of this non-Lorentz-invariant dressing in the spin chain continuum limit is closely related to certain features of the massless case already discussed by one of us.[18] The sine-Gordon model can be formulated in terms of two momentum space cutoffs—Λ limits the maximum particle momentum, Λ' is a momentum space cutoff on the interaction. In the usual field-theoretic formulation, Λ' is taken infinite from the beginning—a local interaction is used. In the spin chain limit, on the other hand, Λ and Λ' are locked together—both being equal to an inverse lattice spacing. We have shown[18] that in the Hartree-Fock contribution to the self-energy, these limits $\Lambda \to \infty$, $\Lambda' \to \infty$ do not commute. It appears, however, that only the limiting velocity is affected by taking the limits differently. In any case, the dressed equations we analyze in this paper arise in both the spin chain limit and the more direct continuum SG analysis, because they involve only the dressed dispersion curves and phase shifts.

B. Thermodynamic equations for general values of the coupling

The TS equations describing *XXZ* and *XYZ* thermodynamics are summarized in Appendix A, and those for the SG system are formally identical.

Minimizing the free energy with respect to the density function ρ_j (for the jth string) gives a set of coupled nonlinear equations for the $\eta_j (\eta_j = \rho_j^h/\rho_j$, ρ_j^h is the density of unoccupied states)

$$\ln\eta_j = -\frac{Aa_j}{T} + \sum_k (-1)^{r(k)} T_{jk} * \ln(1+\eta_k^{-1}) \quad . \tag{2.4}$$

Here $Aa_j(x)$ is the bare dispersion curve for a j string, $(-1)^{r(k)} T_{jk}$ is the bare phase shift between the j and the k string. To find the thermodynamic properties of the system, it is necessary to solve these equations for $\eta_1(x)$, from which the free energy follows:

$$\frac{F}{N} = -2\pi J \frac{\sin\omega}{\omega} \int a_1(x) s_1(x)\, dx - T \int \ln[1+\eta_1(x)] s_1(x)\, dx \quad , \tag{2.5}$$

where $a_1(x)$ and $s_1(x)$ are known functions given in Appendix A, and $\omega = \pi - \mu$.

The problem is that even at low temperatures, the coupled equations (2.4) are not in a convenient form for solution as a result of the presence of the Fermi sea of filled negative energy states ($j = \nu_1$ in the TS notation). This becomes evident on examining the log terms in the sum on the right-hand side of (2.4). For $k < \nu_1$ the strings correspond to positive-energy excitations and η_k^{-1} goes to zero at zero temperature suggesting that an iterative procedure might work. However, $\eta_{\nu_1}^{-1}$ becomes infinite at zero temperature—the Fermi sea becomes fully occupied. The physical significance of this term in (2.4) is clear in the zero-temperature limit. Writing $\ln\eta_j = \epsilon_j/T$, (2.4) in this limit is the equation for the energy of an excitation from the ground state—the first term on the right-hand side is the bare energy (divided by T), the second term corresponds to the dressing caused by backflow in the Fermi sea. The obvious strategy is to rewrite the Eqs. (2.4) in terms of dressed excitations. This is accomplished by putting

$$\ln(1+\eta_{\nu_1}^{-1}) = \ln(1+\eta_{\nu_1}) - \ln\eta_{\nu_1} \tag{2.6}$$

then taking the $\ln\eta_{\nu_1}$ term to the left-hand side in the Eqs. (2.4). In this way, the ν_1 equation gives $\ln\eta_{\nu_1}$ in terms of $\ln(1+\eta_k^{-1})$ for $k \neq \nu_1$, and $\ln(1+\eta_{\nu_1})$, all small terms at low temperatures. This expression for $\ln\eta_{\nu_1}$ is then put into the other equations, so that they express $\ln\eta_k$ for all k in terms of $\ln(1+\eta_l^{-1})$, $l \neq \nu_1$, and $\ln(1+\eta_{\nu_1})$, making low-temperature iteration possible.

The details of this transformation are given in Appendix C for the special values of μ examined in Sec. II C. The general form of the result can be found in Takahashi.[3] It is evident that since after the transformation, the log terms all go to zero at $T=0$, the first term on the right-hand side (corresponding to $-Aa_j/T$ in the bare equation) must be the dressed dispersion curve. Also, the functions corresponding to T_{jk} for the dressed case must be the dressed phase shifts. In fact, the argument is quite general, and the thermodynamics of any BA system with a Fermi sea can be formulated in terms of dressed excitations—a convenient way to analyze low-temperature properties.[19] (Of course, one must be careful to include *all* dressed excitations—as discussed above the DHN excitations are not sufficient for general coupling.)

C. Thermodynamic equations for special values of the coupling

For rational values of the coupling parameter μ/π, the Eqs. (2.4) can be simplified in two distinct ways.

First, for μ/π rational, some ν_j in (A1) is infinite and in (A3) and (A6) some m_i becomes infinite. In the formulation (A6), the final set of equations $m_i \leq j < \infty$ turns out to be rather simple because the function s_i is for this set a δ function, the convolutions become multiplications, and the equations can be solved algebraically.

Second, following TS, one can simply assume that for μ/π rational only strings up to a certain length need be counted, giving a finite set of coupled equations. TS showed that, at least in some cases, this assumption leads to the same results as the algebraic analysis mentioned above.

In this section, we examine these two simplifications for the special values $\mu=[(n-1)/n]\pi$. The first follows naturally from the general case in the limit $\nu_i \to \infty$. We believe our analysis demonstrates that the second is mathematically equivalent to the first, justifying the assumption of TS. In other words, for the special values $\mu=[(n-1)/n]\pi$, an exact analysis of the system is based on a series of coupled equations for the density functions of DHN excitations, corresponding to the analysis of Currie *et al.*[5]

The rest of the section is a detailed discussion of how the simplifications come about as μ tends to a special value $[(n-1)/n]\pi$. It is first necessary to catalog the allowed string lengths and parities, using (A1) and (A2):

$$p_0=\frac{\pi}{\pi-\mu},\quad \frac{1}{p_0}=\frac{1}{\nu_{1}+}\frac{1}{\nu_{2}+}\cdots \ .$$

Taking the limit $\nu_1=n$, and $\nu_2 \to \infty$, we have $p_0=n$, $p_1=1$, $p_2=0$; $y_{-1}=0$, $y_0=1$, $y_1=n$, $y_2=\infty$, and $m_0=0$, $m_1=n$, $m_2=\infty$. The allowed n_j's and parities are then $i=0$:

$$n_1=1^+,\quad n_2=2^+,\ \ldots,\ n_{n-1}=(n-1)^+ \ ;$$

$i=1$:

$$n_n=1^-,\quad n_{n+1}=(n+1)^+,\ n_{n+2}=(2n+1)^-,\ \ldots \ ;$$

$i=2$:

$$n_\infty=n^+ \ .$$

There are no other string lengths corresponding to normalizable wave functions. Recalling that the spacing between members of a string is $2(\pi-\mu)$, and the width of the first zone is 2π, the $i=0$ sequence all fit inside the first zone. The first string in the $i=1$ sequence, the one-member string $n_n=n_{\nu_1}=1^-$, on the $i\pi$ line, corresponds to a particle in the Fermi sea. The second $i=1$ string, $(n+1)^+$ is centered about the real axis with its end members moving to the $i\pi$ line as $\nu_2 \to \infty$. The third $i=1$ string is centered about the $i\pi$ line, with its end members going to the $-i\pi$ and $3i\pi$ lines in the limit. The $i=2$, $n_\infty=n^+$ string is a ghost—for $\nu_2 \to \infty$ its $n\beta_j$'s are such that e^{β_j} are uniformly spaced around the unit circle (with some overall scaling factor) so that the string energy, momentum, and phase shifts, all of which depend on sums over these numbers, are identically zero.

From the definitions of $s_i(x)$ and $d_i(x)$ in (A4), in the limit $\nu_2 \to \infty$ ($p_2 \to 0+$) we find $s_2(x) \to \frac{1}{2}\delta(x)$ and $d_1(x) \to \frac{1}{2}\delta(x)$, so the convolution equations (A6) corresponding to the $i=1$ series above are trivial.

A picture of what is going on as $\nu_2 \to \infty$ might be constructed along the following lines. Consider the $i=1$ $(n+1)^+$ string, which for finite ν_2 fits inside the first zone, but as $\nu_2 \to \infty$ its end members move toward the $\pm i\pi$ lines. The phase shifting between the $(n+1)^+$ string and the 1^- excitations (those on the $i\pi$ line) is such as to induce an extra density of 1^- states near the $(n+1)^+$ string, the rapidity range over which the extra states are induced being of the same magnitude as the distance of the end member of the $(n+1)^+$ from the $i\pi$ line, so as $\nu_2 \to \infty$ the induced phase space tends to a δ function. In a similar way, in this limit all the $i=1$ strings induce only local changes in available phase space for other $i=1$ strings. In fact, this picture is an unnecessarily complicated view of the limit $\nu_2 \to \infty$. This is most evident in the case $\nu_1=2$ and $\nu_2=\infty$, where the above analysis in terms of an infinite sequence of $i=1$ strings gives the correct result (see Appendices E and H of TS) but actually the system is just a noninteracting fermion gas for $\nu_1=2$ and $\nu_2=\infty$! In terms of the bare phase-shift function (discussed in detail in I)

$$\phi(\beta)=-i\ln\left[\frac{\sinh\frac{1}{2}(\beta-2i\mu)}{\sinh\frac{1}{2}(\beta+2i\mu)}\right]$$

for $\mu \neq \frac{1}{2}\pi$ there is a cut from $\beta=2i\mu$ to $\beta=-2i\mu$. For $\mu < \frac{1}{2}\pi$ but close to it, the end points of the cut are close to the $i\pi$ line and account for the extra density of states. For $\mu=\frac{1}{2}\pi$, the end points coincide and the cut vanishes.

For higher ν_1, an analogous but less trivial simplification takes place as $\nu_2 \to \infty$. We examine the particular case $\nu_1=5$, which exhibits all the features of higher values. Again, the convolutions between $i=1$ strings become trivial, but as before, the $i=1$ strings are not actually necessary at $\nu_2=\infty$. This can be seen by examining the allowed strings:

$1^+, 2^+, 3^+, 4^+, 1^-, 6^+, 11^-, \ldots, 5^+$. The 5^+ is the ghost and can be ignored. Consider now the 11^-. Since points in rapidity space are equivalent modulo $2\pi i$, its members can all be placed in the first zone, and we find that $11^- = 6^+ + 4^+ + 1^-$. (This factorization is not true for general coupling of course—the 4^+ would be displaced from the symmetric position about the real axis.) The higher strings factorize similarly $16^+ = 6^+ + 6^+ + 4^+$, etc., and in fact $6^+ = 4^+ + 1^- + 1^-$ so the only distinct entities are 1^+, 2^+, 3^+, 4^+ and 1^-. Furthermore, the phase shifts between 4^+ and $1^+, 2^+, 3^+$ are just minus those between a 1^- and $1^+, 2^+, 3^+$, and the $4^+, 4^+$ phase shift is the same as the $1^-, 1^-$, both being equal to minus the $4^+, 1^-$ phase shift. (There is a simple reason for this—the set $4^+ + 1^-$ is just a displaced 5^+ ghost, having identically zero-phase shifts.) It follows from this that in the thermodynamic BA equations, 4^+ string and holes in the 1^- Fermi sea must have identical distributions in rapidity space.

The above argument establishes that for $\mu = 4/5\pi$ there are only four distinct density functions η_j, since η_4 (for 4^+ strings) is identical to η_5^{-1} (for 1^- holes). Thus there are only four equations in the series (2.4). These equations are written out explicitly for the *XXZ* case in Appendix C [Eqs. (C2)—the last two are identical]. In that Appendix, we also show how to derive the dressed equations, and how to take the SG limit. This gives the equations solved numerically in Sec. III.

III. NUMERICAL ANALYSIS

In this section, we present the results of a numerical analysis of the set of nonlinear integral equations describing the thermodynamics of the sine-Gordon system for $\mu = [(n-1)/n]\pi$, $n = 5, 10$. The relevant equations, in terms of dressed excitations, are given in Appendix C, Eqs. (C6) with the α_i's given by (C11) and (C13).

To solve Eqs. (C6) numerically, we define $hj = ln(1+\eta_j^{-1})$ and transform them as follows:

$$h_j = \ln[1+\exp(-E_j^0/T \cdots -\alpha_l * h_k \cdots)] \;, \qquad j = 1, \ldots, n-2 \;, \quad (3.1)$$

$$h_{n-1} = \ln[1+\exp(-E_s^0/T \cdots -\alpha_l * h_k \cdots)] \;,$$

where $\cdots \alpha_l * h_k \cdots$ denotes the convolutions on the right-hand side of Eqs. (C6).

Equations (3.1) consititue a set of coupled nonlinear integral equations that can be solved by iteration. Once we find the h_j's we can find the free-energy density using (C6′), (C12), and (C13).

$$F = -\sum_{j=1}^{n-1} T \int_{-\Lambda}^{+\Lambda} \frac{1}{2\pi} 2\sin\left[j\frac{\pi(\pi-\mu)}{2\mu}\right] \times \cosh\left[\frac{\pi}{2}\frac{\beta}{\mu}\right] h_j d\left[\frac{\pi\beta}{2\mu}\right] \qquad (3.2)$$

The energy, entropy, and specific heat can be found using the following thermodynamic identities

$$E = -T^2 \frac{\partial}{\partial T}\left[\frac{F}{T}\right], \quad S = \frac{E-F}{T}, \quad C = \frac{\partial E}{\partial T}$$

by direct analytical differentation with respect to temperature of (3.1) and (3.2). Defining $u_j = T^2 \partial h_j / \partial T$, $\hat{u}_j = \partial u_j / \partial T$, we obtain two more sets of integral equations that we also solve by iteration:

$$u_j = (1-e^{-h_j})(E_j^0 - \cdots -\alpha_l * u_k - \cdots) \;, \qquad j = 1, \ldots, n-2 \;, \quad (3.3)$$

$$u_{n-1} = (1-e^{h_{n-1}})(E_s^0 - \cdots -\alpha_l * u_k \cdots) \;,$$

$$E = \sum_{j=1}^{n-1} \int_{-\Lambda}^{+\Lambda} \frac{1}{2\pi} 2\sin\left[j\frac{\pi(\pi-\mu)}{2\mu}\right] \times \cosh\left[\frac{\pi}{2}\frac{\beta}{\mu}\right] u_j d\left[\frac{\pi\beta}{2\mu}\right] \;, \qquad (3.4)$$

and

$$\hat{u}_j = \frac{1}{T^2}\frac{u_j^2}{e^{h_j}-1} + (1-e^{-h_j})(- \cdots -\alpha_l * \hat{u}_k - \cdots) \;, \qquad (3.5)$$

$$C = \sum_{j=1}^{n-1} \int_{-\Lambda}^{+\Lambda} \frac{1}{2\pi} 2\sin\left[j\frac{\pi(\pi-\mu)}{2\mu}\right] \times \cosh\left[\frac{\pi}{2}\frac{\beta}{\mu}\right] \hat{u}_j d\left[\frac{\pi\beta}{2\mu}\right] \;. \qquad (3.6)$$

The three sets of equations (3.1), (3.3) and (3.5) were solved by iteration so that h_j, u_j, $\hat{u}_j$ were determined with a precision of 10^{-3}. Each function was represented in rapidity space, β, with approximately 50 points and Simpson's rule was used for the numerical integrations. The cutoff Λ was chosen so that all contributions in the integrals were included (and the results were independent of cutoff). The calculation was performed on a VAX 11/780 computer. In Fig. 1 we present the results of the specific heat for $\mu = \frac{4}{5}\pi$ and $\frac{9}{10}\pi$ after subtracting the specific heat of a free-boson gas;

$$C_{\text{phonon}} = \frac{1}{T^2}\int_{-\infty}^{+\infty} \frac{\omega^2}{4\sinh^2(\omega/2T)} \frac{dk}{2\pi}$$

with dispersion relation

$$\omega^2 = (m_1^2 + k^2)^{1/2}$$

and mass

$$m_1 = 2\sin[\pi(\pi-\mu)/2\mu] \;.$$

The difference in specific heat has a maximum around a temperature of 0.4 in soliton mass units and goes to zero as $T \to +\infty$. Therefore at high temperature the total specific heat goes asymptotically to a

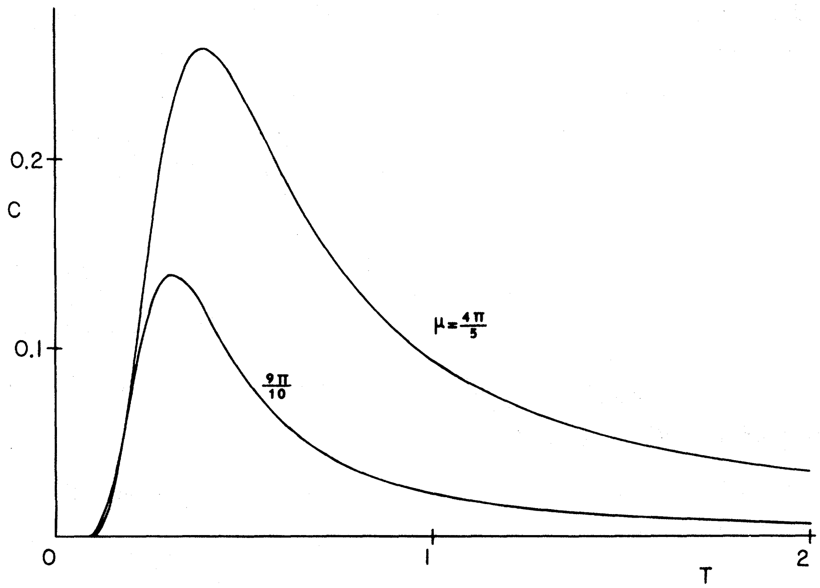

FIG. 1. Specific heat vs temperature for SG model at $\mu=\frac{4}{5}\pi$, $\frac{9}{10}\pi$ (temperature in soliton mass units and the noninteracting phonon specific heat has been subtracted).

straight line passing through the origin with slope $\frac{1}{3}\pi$ corresponding to the specific heat of a free-phonon gas with dispersion relation $\omega=k$. (The sine-Gordon potential term is completely washed out.) At low temperatures we obtain the correct exponential behavior given by the dressed mass of the phonon for $\mu>\frac{3}{4}\pi$ and the soliton mass for $\mu=\frac{2}{3}\pi$. In Fig. 2 we show the population $P1=\rho_1/(\rho_1+\rho_1^h)=1-e^{-h_1}$ as a function of rapidity β, of string $j=1$ (particles on the real axis) for four different temperatures, for $\mu=\frac{4}{5}\pi$.

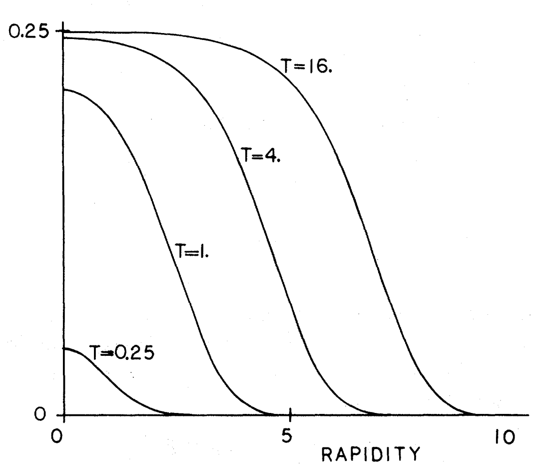

FIG. 2. Population of the $j=1$ string vs rapidity for a series of temperatures at $\mu=\frac{4}{5}\pi$. (Temperature in soliton mass units.)

We notice that the population of the $j=1$ string, goes to 0.25 at high temperatures. In fact, the high-temperature limits for the population of the different strings are of the form

$$\frac{\rho_j}{\rho_j+\rho_j^h}\underset{T\to+\infty}{\longrightarrow}\frac{1}{(j+1)^2}\ ,\quad j=1,\ldots,n-2\ ,$$

$$\frac{\rho_{n-1}}{\rho_{n-1}+\rho_{n-1}^h}\underset{T\to+\infty}{\longrightarrow}\frac{1}{n}\ .$$

This limit follows from Eqs. (A6) assuming $\ln(1+n_j)$ approximately constant near zero rapidity, which is correct for $T\to+\infty$.

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APPENDIX A

We summarize here some of the results of Takahashi and Suzuki for *XXZ* and *XYZ* spin chains. As all the integral equations involve summing over allowed (normalizable) strings, it is necessary to state the orders and parities of allowed strings. [Strings are centered about the real axis (positive parity) or $\mathrm{Im}\,\alpha=\pi$ (negative parity).]

Following TS, we define series of real numbers p_i and integers ν_i, m_i, and y_i by

$$p_0=\pi/\omega,\quad \omega=\pi-\mu=2\zeta,\quad p_1=1\ ,$$

$$\nu_i=\left[\frac{p_{i-1}}{p_i}\right],\quad p_i=p_{i-2}-p_{i-1}\nu_{i-1}\ ,$$

$$m_0=0,\quad m_i=\sum_{k=1}^{i}\nu_k\ , \tag{A1}$$

$$y_{-1}=0,\quad y_0=1,\quad y_1=\nu_1\ ,$$

$$y_2=\nu_1\nu_2+1,\ \ldots,\ y_i=y_{i-2}+\nu_i y_{i-1}\ .$$

Thus $\omega/\pi=(1/\nu_1+)(1/\nu_2+)\cdots$. Then the order and parity of all normalizable strings are given by

$$n_j=y_{i-1}+(j-m_i)y_i$$

$$\text{for } m_i\le j<m_{i+1},\quad j=1,2,\ldots$$

$$v_1=+1,\quad v_{m_1}=-1\ , \tag{A2}$$

$$v_j=\exp\left[\pi i\left(\frac{(n_j-1)}{\pi}\omega\right)\right]$$

$$\text{for } j\neq 1,m_1\ .$$

TS show that the BA boundary condition equations for the XXZ system can be written

$$\rho_j+\rho_j^h=s_i*(\rho_{j-1}^h+\rho_{j+1}^h)\ ,$$

$$m_{i-1}\le j\le m_i-2\ , \tag{A3}$$

$$\rho_j+\rho_j^h=s_i*\rho_{j-1}^h+d_i*\rho_j^h-s_{i+1}*\rho_{j+1}^h\ ,$$

$$\text{for } j=m_i-1\ ,$$

where ρ_j and ρ_j^h are the densities of j strings and j string holes,

$$s_i(x)=\frac{1}{4p_i}\operatorname{sech}\frac{\pi x}{2\pi}\ ,$$

$$d_i(x)=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{e^{ikx}\cosh[(p_i-p_{i+1})k]}{2\cosh p_ik\cosh p_{i+1}k} \tag{A4}$$

and the asterisk denotes a convolution from $-\infty$ to ∞. (We use TS notation.) Minimizing the free energy with respect to ρ_j gives the following equations for the $\eta_j(\rho_j^h/\rho_j)$:

$$\ln\eta_j=-\frac{A}{T}a_j+\sum_{k=1}^{\infty}(-1)^{r(k)}T_{jk}*\ln(1+\eta_k^{-1})\ , \tag{A5}$$

where $A=2\pi J_z\sin\omega/\omega$, $r(j)$ is defined by $m_{r(j)}\le j<m_{r(j)+1}$,

$$T_{jk}=a(x;|n_j-n_k|,v_jv_k)+a(x;n_j+n_k,v_jv_k)$$

$$+2\sum_{i=1}^{\min(n_j,n_k)-1}a(x;|n_j-n_k|+2i,v_jv_k)$$

for $j\neq k$, if $j=k$ the first term is omitted.

$$a(x,n_j,v_j)=-\frac{1}{2\pi}\frac{d}{dx}t_j(x)\ ,$$

$$t_j(x)=\begin{cases}0 & \text{for } n/p_0 \text{ is an integer}\\ 2v\tan^{-1}\{[\cot(n\pi/2p_0)]^v\tanh(\pi x/2p_0)\} & \text{otherwise}\ ,\end{cases}$$

which can be rewritten [using (A3)] in the form

$$\ln(1+\eta_0)=-2\pi J\sin\omega\frac{\delta(x)}{\omega T}\ ,$$

$$\ln\eta_j=(1-2\delta_{m_{i-1},j})s_i*\ln(1+\eta_{j-1})+s_i*\ln(1+\eta_{j+1})$$

$$\text{for } m_{i-1}\le j<m_i-2\ ,$$

$$\ln\eta_j=(1-2\delta_{m_{i-1},j})s_i*\ln(1+\eta_{j-1})$$

$$+d_i*\ln(1+\eta_j)+s_{i+1}*\ln(1+\eta_{j+1}) \tag{A6}$$

$$\text{for } j=m_i-1\ ,$$

where the free energy

$$\frac{F}{N}=-2\pi J\frac{\sin\omega}{\omega}\int_{-\infty}^{+\infty}a_1(x)s_1(x)\,dx$$

$$-T\int_{-\infty}^{+\infty}\ln[1+\eta_i(x)]s_1(x)\,dx\ . \tag{A7}$$

Here

$$a_1(x)=\frac{1}{2p_0}\frac{\sin\pi/p_0}{\cos\pi x/p_0-\cos\pi/p_0}\ . \tag{A8}$$

The above sets of equations, then, give a complete description of the thermodynamics of the XXZ spin chain (we have for simplicity taken zero external field). For the XYZ spin chain (with N sites) the following changes are necessary:

(a) Rex is restricted to $[-Q,Q]$ where $Q=K_l'/\zeta$

$$(J_x{:}J_y{:}J_z=\text{cn}(2\zeta,l){:}\text{dn}(2\zeta,l){:}1)\ , \tag{A9}$$

(b) $p_0=K_l/\zeta$;

(c) $s_i(x)$ and $d_i(x)$ are replaced by

$$\tilde{s}_i(x)=\sum_{j=-\infty}^{\infty}s_i(x+2jQ)\ ,$$

$$\tilde{d}_i(x)=\sum_{j=-\infty}d_i(x+2jQ)\ .$$

In other words, the XYZ model has a periodicity in the real direction as well as retaining that in the imaginary direction, so elliptic functions arise naturally. In the XYZ model,

$$\tilde{a}_1(x)=\frac{\zeta}{\pi}\left[Z(\zeta)+\frac{\text{sn}\zeta\,\text{cn}\zeta\,\text{dn}\zeta}{\text{sn}^2\zeta-\text{sn}^2(i\zeta x)}\right]\ , \tag{A10}$$

where $Z(\zeta)$ denotes Jacobi's ζ function of modulus l.

APPENDIX B: THE SG LIMIT OF THE *XYZ* SPIN SYSTEM

In this appendix, we show in detail how the various expressions used by TS for the *XYZ* spin chain go to the appropriate form in the SG limit.

We take the *XYZ* Hamiltonian to be

$$H=-\tfrac{1}{2}\sum_{i=1}^{N}(J_x s_i^x s_{i+1}^x + J_y s_i^y s_{i+1}^y + J_z s_i^z s_{i+1}^z) \quad \text{(B1)}$$

with $J_x{:}J_y{:}J_z = \mathrm{cn}(2\zeta,l){:}\mathrm{dn}(2\zeta,l){:}1$,

$$1>l>0,\quad K_l \geqslant 2\zeta \geqslant 0 \ .$$

(This is the form most widely used. Unfortunately, TS omit the overall factor of $-\frac{1}{2}$. In this appendix, we use their equations and make the appropriate correction at the end.)

The limiting form of the phase shift has already been discussed in I.

Let us consider the bare dispersion curve, from TS (4.5a) and (4.8):

$$E=-\frac{J_z\pi}{\zeta}\,\mathrm{sn}(2\zeta)\,\tilde{a}_1(x) \ ,$$
$$\tilde{a}_1(x)=\frac{\zeta}{\pi}\left(Z(\zeta)+\frac{\mathrm{sn}\zeta\,\mathrm{cn}\zeta\,\mathrm{dn}\zeta}{\mathrm{sn}^2\zeta-\mathrm{sn}^2 i\zeta x}\right) \ , \quad \text{(B2)}$$

where ζ is defined by (B1), and is related to Bergknoff and Thacker's μ and Korepin's ω by

$$2\zeta=\pi-\mu=\omega \ . \quad \text{(B3)}$$

The elliptic functions sn, cn, dn, and Z have modulus l defined by (B1). The variable x is essentially the bare "rapidity" variable.

Let us consider the properties of $\tilde{a}_1$ as a function of x, first for real x. The function $\mathrm{sn}^2 z$ is real for z pure imaginary, with period $2K_l'$, having a double zero at the origin and a double pole at K_l'. Hence for real x, $\tilde{a}_1(x)$ is real and periodic with period $2Q$, where

$$Q=K_l'/\zeta \ , \quad \text{(B4)}$$

having a maximum at the origin and a minimum at Q. This is a dispersion curve for positive-energy bare excitations. The negative-energy bare particles, which constitute the filled Fermi sea in the ground state, fill one period $2Q$ of the line $\mathrm{Im}x=K_l/\zeta$. The function $\tilde{a}_1(x)$ along this line is again real and periodic, but with a minimum at the origin and a maximum at Q.

Since the positive-energy excitations have their minimum energy at Q (and the negative energy ones their maximum) it is evident that in the sine-Gordon limit Q must correspond to the origin. We define the sine-Gordon rapidity in terms of x by shifting the origin to Q, and scaling by -2ζ to coincide with the standard notation:

$$\beta/2\zeta=Q-x \ . \quad \text{(B5)}$$

From the $2Q$ periodicity of the system, the filled Fermi sea can be regarded as lying between $\beta=-2\zeta Q$ and $+2\zeta Q$. If now the cutoff is taken to infinity ($2\zeta Q=2K_l'\to\infty, l\to 0$) the energy near $\beta=0$ has the form

$$E\cong J_z(\sin^2 2\zeta)\tfrac{1}{4}l^2\cosh\beta \ . \quad \text{(B6)}$$

(This refers to the TS Hamiltonian. To derive this expression, note that at $\beta=0$, $\mathrm{sn}^2 i\zeta x$ has a pole. Near $\beta=0$, we use $\mathrm{sn}^2 i\zeta x\cong l^{-2}ns^2 i\beta/2$ for small l.)

We now look at the expression for the bare momentum. From TS equation (4.3a), taking the lattice spacing to be a,

$$ka=-i\ln\frac{H(\zeta(x+i))}{H(\zeta(x-i))} \ . \quad \text{(B7)}$$

Changing variables to β using (B5), and using the same transformations discussed in the appendix of I, with $K\equiv K_l'$ and $K'\equiv K_l$

$$\ln\frac{H(\frac{1}{2}(2K+2i\zeta-\beta))}{H(\frac{1}{2}(2K-2i\zeta-\beta))}=\ln\frac{H_1(\frac{1}{2}(2i\zeta-\beta))}{H_1(\frac{1}{2}(2i\zeta+\beta))}=\ln\left[\theta_2\left(\frac{\pi\zeta}{4K}(2i\zeta-\beta)\right)\Big/\theta_2\left(\frac{\pi\zeta}{4K}(2i\zeta+\beta)\right)\right] \ . \quad \text{(B8)}$$

This is to be evaluated in the limit $K\to\infty$, $q=\exp(-\pi K'/K)\to 1$, so we use (as in I) the transformation

$$\sqrt{-i\tau}\,\theta_2(z|\tau)=\exp(i\tau' z^2/\pi)\,\theta_4(z\tau'|\tau') \ ,$$
$$\tau'=-1/\tau,\quad \tau=\frac{iK'}{K} \quad \text{(B9)}$$

The exponential term contributes $i\zeta\beta/K$. This is analogous to the small term in the phase shift noted in I, symptomatic of the underlying lattice structure, and becoming small in the continuum limit. The other term gives (as $K\to\infty$)

$$ka=\tfrac{1}{4}l^2\sin 2\zeta\sinh\beta \ . \quad \text{(B10)}$$

We turn now to a consideration of the functions describing the dressed system. The zero-temperature dressed excitations energies are written

$$\epsilon_j(x)=-A\,\alpha_j(x),\quad \epsilon_{\nu_1}(x)=A\,\beta(x) \quad \text{(B11)}$$

by Takahashi. The functions α_j and β are the same ones which appear in the thermodynamic equation

(2.4). Here

$$A = \pi J_z \,\mathrm{sn} 2\zeta/\zeta \quad , \tag{B12}$$

$$\beta(x) = \frac{K_{k'}}{2\pi(p_0-1)} \mathrm{dn}\left[\frac{K_{k'}x}{p_0-1}, k\right] \; ,$$
$$\alpha_j(x) = \beta(x + i(p_0 - 1 - j)) + \beta(x - i(p_0 - 1 - j)) \; , \tag{B13}$$

where k is defined by

$$\frac{K_k}{K_{k'}} = \frac{K_l'}{K_l - \zeta}, \quad p_0 = \frac{K_l}{\zeta} \quad . \tag{B14}$$

At $x = Q$,

$$\alpha_j(Q) = \frac{K_{k'}k'}{\pi(p_0-1)} \mathrm{sn}\left[\frac{K_{k'}j}{p_0-1}, k'\right] \; ,$$
$$\beta(Q) = \frac{K_{k'}k'}{2\pi(p_0-1)}, \quad \beta''(Q) = \frac{K_{k'}^3 k^2 k'}{2\pi(p_0-1)^3} \quad . \tag{B15}$$

In the SG limit we have

$$l \to 0, \quad K_l' \to \infty, \quad K_l \to \tfrac{1}{2}\pi \; ,$$
$$k' \to 0, \quad K_k \to \infty, \quad K_k' \to \tfrac{1}{2}\pi \; , \tag{B16}$$
$$K_l' \to \ln\frac{4}{l}, \quad K_k \to \ln\frac{4}{k'} \quad .$$

Thus

$$\tfrac{1}{4}k' = (\tfrac{1}{4}l)^{K_k/K_l'} = (\tfrac{1}{4}l)^{\pi/\pi - 2\zeta} = (\tfrac{1}{4}l)^{\pi/\mu} \; , \tag{B17}$$

also using $2\zeta = \pi - \mu$ and $\mathrm{sn}2\zeta \to \sin\mu$.

In the SG limit the soliton energy gap (for example, in specific heat) is $A\beta(Q)$, the $A\alpha_j$'s correspond to the DHN $s\bar{s}$ bound states in the zero-temperature limit.

The soliton mass is

$$A\beta(Q) = \frac{\pi J_z \,\mathrm{sn}2\zeta}{\zeta} \frac{K_{k'}k'\zeta}{2\pi(K_l - \zeta)} = J_z \sin\mu \frac{\pi}{2\mu} k'$$
$$= J_z \frac{\pi}{2\mu}(\sin\mu) 4(\tfrac{1}{4}l)^{\pi/\mu} \quad . \tag{B18}$$

The $s\bar{s}$ masses are equal to the soliton mass multiplied by the scaling factor $2\sin[j\pi(\pi-\mu)/2\mu]$ found by DHN.

To find the function $\beta(x)$ for arbitrary rapidities in the SG system, we need to evaluate the limit of $\mathrm{dn}[K_{k'}x/(p_0-1), k]$ as $k' \to 0$. The argument

$$\frac{K_{k'}}{K_l - \zeta}\zeta x = \frac{K_k}{K_{l'}}\zeta x = K_k - \frac{K_k}{K_{l'}}\frac{\beta}{2}$$

using (B4) and (B5).

Using $\mathrm{dn}(u + K) = k'\mathrm{nd}u$, and taking the limit $k' \to 0$, so $\mathrm{dn}x \to \mathrm{sech}x$ and $K_k/K_{l'} \to \pi/\mu$, we find

$$A\beta(x) = J_z \frac{\pi}{2\mu}(\sin\mu)\, 4(\tfrac{1}{4}l)^{\pi/\mu} \cosh\frac{\pi\beta}{2\mu} \tag{B19}$$

when expressed in terms of the standard SG rapidity variable β.

The SG limit is defined as $l \to 0$ and $J_z \to \infty$ such that this mass gap is finite. At the same time, the lattice spacing $a \to 0$ and the relationship between a and J_z in the limit is given by requiring the appropriate energy-momentum relationship for the dressed particles, using the expressions found by Johnson, Krinsky, and McCoy (JKM) for the XYZ chain.

For the energy,

$$\Delta E_{\mathrm{JKM}} = -J_z \,\mathrm{sn}(2\zeta, l) \frac{K_1}{K_{l'}} \mathrm{dn}\left[\frac{K_1\phi_1}{\pi}, k_1\right] \quad . \tag{B20}$$

Here

$$K_{l'}(\mathrm{JKM}) \equiv K_{l'}(\mathrm{TS}) \; ,$$
$$K_1(\mathrm{JKM}) \equiv K_k(\mathrm{TS}) \; , \tag{B21}$$

and the JKM Hamiltonian is $\frac{1}{2}$ the TS Hamiltonian. The minimum value of dn above is $k_{1}'(\mathrm{JKM})$ or $k'(\mathrm{TS})$ so it is easy to check that ΔE_{JKM} agrees with ΔE_{TS} discussed above.

The momentum of an elementary excitation is given by JKM as

$$qa = \int_{-k_1}^{k_1\phi_i/\pi} \mathrm{dn}(\phi, k_1)\, d\phi \quad , \tag{B22}$$

where we have written the lattice spacing a explicitly. Switching to TS notation $k_1 \to k$ and $K_1 \to K$ and changing variables to $\psi_i = \pi + \phi_i$,

$$qa = \int_0^{k\psi_i/\pi} \mathrm{dn}(\psi - K, k)\, d\psi \quad . \tag{B23}$$

Using $\mathrm{dn}(u - K) = k'\mathrm{nd}u \approx k'\cosh u$ in the SG limit,

$$qa = k' \sinh\frac{K_k\psi_i}{\pi} = 4\left[\frac{l}{4}\right]^{\pi/\mu} \sinh\frac{\pi\beta}{2\mu} \quad . \tag{B24}$$

Thus to have $E^2 = m^2 + q^2$ for the dressed excitations,

$$\frac{1}{a} = -J_z \frac{\pi}{2\mu}\sin\mu \quad .$$

APPENDIX C: DERIVING THE DRESSED EQUATIONS FROM THE BARE EQUATIONS FOR $\mu = \frac{4}{5}\pi$

We have established in Sec. II that for $\mu = \frac{4}{5}\pi$ there are five allowed strings, $i = 1, 2, 3, 4$ being strings of length 1, 2, 3, 4, centered on the real axis, $i = 5$ being the string 1^-, a single point on the $i\pi$ line.

We shall work here with the XXZ model, and show at the end how to generalize to XYZ and hence the SG case. The thermodynamics equations for the bare densities of particles are given by (A5) where now $j,k = 1, \ldots, 5$. It is convenient to Fourier transform the equations so that the convolutions become multiplications.

The Fourier transforms of the functions a_j are

$$a_j(k)=\frac{\sinh(5-j)k}{\sinh 5k} \quad . \tag{C1}$$

Substituting this into the T_{jk} defined below (A5) gives the following series of equations:

$$\ln\eta_1=-\frac{Aa_1}{T}+a_2\ln(1+\eta_1^{-1})+(a_1+a_3)\ln(1+\eta_2^{-1})+(a_2+a_4)\ln(1+\eta_3^{-1})+a_3\ln(1+\eta_4^{-1})+a_3\ln(1+\eta_5^{-1}) \; ,$$

$$\ln\eta_2=-\frac{Aa_2}{T}+(a_1+a_3)\ln(1+\eta_1^{-1})+(2a_2+a_4)\ln(1+\eta_2^{-1})+(2a_3+a_1)\ln(1+\eta_3^{-1})$$
$$+(a_2+a_4)\ln(1+\eta_4^{-1})+(a_2+a_4)\ln(1+\eta_5^{-1}) \; ,$$

$$\ln\eta_3=-\frac{Aa_3}{T}+(a_2+a_4)\ln(1+\eta_1^{-1})+(a_1+2a_3)\ln(1+\eta_2^{-1})+(a_4+2a_2)\ln(1+\eta_3^{-1})$$
$$+(a_3+a_1)\ln(1+\eta_4^{-1})+(a_3+a_1)\ln(1+\eta_5^{-1}) \; , \tag{C2}$$

$$\ln\eta_4=-\frac{Aa_4}{T}+a_3\ln(1+\eta_1^{-1})+(a_2+a_4)\ln(1+\eta_2^{-1})+(a_1+a_3)\ln(1+\eta_3^{-1})+a_2\ln(1+\eta_4^{-1})+a_2\ln(1+\eta_5^{-1}) \; ,$$

$$\ln\eta_5=\frac{Aa_4}{T}-a_3\ln(1+\eta_1^{-1})-(a_2+a_4)\ln(1+\eta_2^{-1})-(a_1+a_3)\ln(1+\eta_3^{-1})-a_2\ln(1+\eta_4^{-1})-a_2\ln(1+\eta_5^{-1}) \; .$$

In deriving the sums over a_i's appearing here we have used such properties as $a_6=-a_4$, evident from (C1). We see here (as discussed in Sec. II) that

$$\ln\eta_4=-\ln\eta_5 \tag{C3}$$

so these are really only four unknown different density functions.

The above equations are unsuitable for low-temperature iteration because although $\ln(1+\eta_i^{-1})\to 0$ for $i=1,2,3,4$ this is not so for $i=5$—the Fermi sea term. To get rid of this term, we write

$$\ln(l+\eta_5^{-1})=\ln(1+\eta_4)=\ln(1+\eta_4^{-1})+\ln\eta_4 \tag{C4}$$

in Eqs. (C2).

The fourth equation then becomes

$$(1-a_2)\ln\eta_4=-\frac{Aa_4}{T}+a_3\ln(1+\eta_1^{-1})+(a_2+a_4)\ln(1+\eta_2^{-1})+(a_1+a_3)\ln(1+\eta_3^{-1})+3a_2\ln(1+\eta_4^{-1}) \; . \tag{C5}$$

This expression for $\ln\eta_4$ is then substituted in the first three equations of (C2), giving four equations for n_i, $i=1,\ldots,4$, in a form suitable for low-temperature iteration. It is straightforward although tedious to verify that this procedure gives

$$\ln\eta_1=-\frac{A}{T}\alpha_1+\alpha_2\ln(1+\eta_1^{-1})+(\alpha_1+\alpha_3)\ln(1+\eta_2^{-1})+(\alpha_2+\alpha_4)\ln(1+\eta_3^{-1})+2\alpha_3\ln(1+\eta_4^{-1}) \; ,$$

$$\ln\eta_2=-\frac{A}{T}\alpha_2+(\alpha_1+\alpha_3)\ln(1+\eta_1^{-1})+(2\alpha_2+\alpha_4)\ln(1+\eta_2^{-1})+(\alpha_1+3\alpha_3)\ln(1+\eta_3^{-1})+2(\alpha_2+\alpha_4)\ln(1+\eta_4^{-1}) \; ,$$

$$\ln\eta_3=-\frac{A}{T}\alpha_3+(\alpha_2+\alpha_4)\ln(1+\eta_1^{-1})+(\alpha_1+3\alpha_3)\ln(1+\eta_2^{-1})+(3\alpha_2+2\alpha_4)\ln(1+\eta_3^{-1})+(2\alpha_1+4\alpha_3)\ln(1+\eta_4^{-1}) \; ,$$

$$\ln\eta_4=-\frac{A}{T}\beta+\alpha_3\ln(1+\eta_1^{-1})+(\alpha_2+\alpha_4)\ln(1+\eta_2^{-1})+(\alpha_1+2\alpha_3)\ln(1+\eta_3^{-1})+(2\alpha_2+\alpha_4)\ln(1+\eta_4^{-1}) \; . \tag{C6}$$

Here the functions α_j and β are given by

$$\alpha_j(k)=\frac{\cosh(4-j)k}{\cosh 4k},\quad \beta(k)=\frac{1}{2\cosh 4k} \quad . \tag{C7}$$

A useful identity in deriving (C6) is

$$\alpha_j=a_j+\frac{a_3a_{5-j}}{1-a_2} \quad . \tag{C8}$$

Also the expression for the free energy

$$\frac{F}{N}=-A\int_{-\infty}^{+\infty}s_1a_1\,dx-T\int_{-\infty}^{+\infty}s_1\ln(1+\eta_1)\,dx$$

is given in terms of $\ln(1+\eta_1)$ which diverges as $T\to 0$. We can also transform this expression in terms of density functions $\ln(1+\eta_j^{-1})$, $j=1,\ldots,4$. Using the first of dressed equations (C6) (after Fourier transforming)

$$\frac{F}{N}=-A\int_{-\infty}^{+\infty}s_1a_1\,dk-T\int_{-\infty}^{+\infty}[s_1\ln\eta_1+s_1\ln(1+\eta_1^{-1})]\,dk$$

$$=-A\int_{-\infty}^{+\infty}s_1a_1\,dk-T\int_{-\infty}^{+\infty}s_1\left[-\frac{A}{T}\alpha_1+\alpha_2\ln(1+\eta_1^{-1})+(\alpha_1+\alpha_3)\ln(1+\eta_2^{-1})\right.$$

$$\left.+(\alpha_2+\alpha_4)\ln(1+\eta_3^{-1})+2\alpha_3\ln(1+\eta_4^{-1})\right]+s_1\ln(1+\eta_1^{-1})\,dk$$

and after combining terms

$$\frac{F}{N}=-A\int_{-\infty}^{+\infty}s_1(a_1-\alpha_1)\,dk-T\int_{-\infty}^{+\infty}(s_1\alpha_2+s_1)\ln(1+\eta_1^{-1})+s_1(\alpha_1+\alpha_3)\ln(1+\eta_2^{-1})$$

$$+s_1(\alpha_2+\alpha_4)\ln(1+\eta_3^{-1})+2s_1\alpha_3\ln(1+\eta_4^{-1})\,dk \quad .$$

Using the identities $s_1(k)[\alpha_{j-1}(k)+\alpha_{j+1}(k)]=\alpha_j(k)$ we obtain

$$\frac{F}{N}=\text{const}-T\sum_{j=1}^{n-1}\int_{-\infty}^{+\infty}\alpha_j\ln(1+\eta_j^{-1})\,dx \quad (n=5) \quad . \tag{C6$'$}$$

Having established the transformation from the bare equations (C2) to the dressed equations (C6) for the *XXZ* model, it is easy to generalize to the *XYZ* case. As outlined in Appendix A, the convolutions are now over $[-Q,Q]$ instead of the whole real line, and $a_i(x)$ is replaced by

$$\tilde{a}_i(x)=\sum_{j=-\infty}^{\infty}a_i(x+2jQ) \quad . \tag{C9}$$

The functions $\tilde{\alpha}_i(x)$ and $\tilde{\beta}(x)$ are similarly defined, and the particle densities are nonzero only in a single period $2Q$ of these functions. Thus a Fourier-series analysis is appropriate for Eqs. (C2). Defining the nth Fourier coefficient by

$$\tilde{a}_i(n)=\frac{1}{2\pi}\int_{-Q}^{Q}\tilde{a}_i(x)e^{2\pi i n/Q}dx \quad ,$$

from (C9),

$$a_i(n)=\frac{1}{2\pi}\int_{-\infty}^{\infty}a_i(x)e^{2\pi i n/Q}dx=a_i(k) \quad , \tag{C10}$$

where $k=2\pi n/Q$. That is to say, the Fourier coefficients in the series for $\tilde{a}_i$ are identical to the Fourier transforms of the functions a_i at the corresponding k values. Hence identifies such as (C8) for the Fourier transforms of a_i and α_i also hold for the Fourier series coefficients of $\tilde{a}_j$ and $\tilde{\alpha}_i$ and (C6) follows.

To find the equations for the sine-Gordon system one must of course take the Eqs. (C6) for *XYZ* in the limit discussed in detail in Appendix B. It is important to note that in the SG limit, the α_i appearing in the *phase shifts* above go to their *XXZ* limit,

$$\alpha_j(\text{phase shift})\to-\frac{1}{2\pi i}\frac{d}{d\beta}\ln\frac{\tan\frac{1}{2}[i\pi(\beta-\beta')/2\mu-j\pi(\pi-\mu)/2\mu]}{\tan\frac{1}{2}[i\pi(\beta-\beta')/2\mu+j\pi(\pi-\mu)/2\mu]}$$

$$=\frac{1}{\mu}\frac{\cosh[(\pi/2)(\beta-\beta')/\mu]\sin[j\pi(\pi-\mu)/2\mu]}{\cosh[\pi(\beta-\beta')/\mu]-\cos[j\pi(\pi-\mu)/\mu]} \quad , \tag{C11}$$

whereas the α_i and β in the leading terms on the right-hand side of (C6) go to SG dispersion curves

$$\alpha_j(\text{dispersion term}) \rightarrow \frac{\pi-\mu}{\mu}\left(\tfrac{1}{4}l\right)^{\pi/\mu} 2\sin\left[j\frac{\pi(\pi-\mu)}{2\mu}\right]\cosh\left[\frac{\pi\beta}{2\mu}\right] ,$$

$$\beta \rightarrow \frac{\pi-\mu}{\mu}\left(\tfrac{1}{4}l\right)^{\pi/\mu}\cosh\left[\frac{\pi}{2}\frac{\beta}{\mu}\right] . \tag{C12}$$

The reason for this difference is discussed in detail in Appendix B. Taking the unit of energy to be the soliton mass, $[(1/a)4(\frac{1}{4}l)^{\pi/\mu}=1,\ a\rightarrow 0,\ l\rightarrow 0]$, the expression (C12) becomes

$$-A\,\alpha_j = E_j^0 = m_j \cosh\left[\frac{\pi\beta}{2\mu}\right] , \quad -A\,\beta = E_s^0 = \cosh\left[\frac{\pi\beta}{2\mu}\right] , \tag{C13}$$

where $m_j = 2\sin[j\pi(\pi-\mu)/2\mu]$ is the jth phonon mass. The equations we have analyzed numerically were those given by putting (C13) and (C11) into (C6).

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