PHYSICAL REVIEW B VOLUME 37, NUMBER 11 15 APRIL 1988-I

Fluctuation properties of thermal solitons

Nikos Theodorakopoulos*
Institut für Physik der Universität Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Erich W. Weller
Max-Planck-Institut für Festkörperforschung, Postfach 80 06 65, D-7000 Stuttgart 80, Federal Republic of Germany

(Received 28 August 1987)

The thermodynamic properties of soliton-bearing systems can be obtained from the statistics of their soliton components, which reflect restrictions on phase space due to interactions. Going beyond the established agreement of the free energy with transfer-integral results, we have successfully tested first derivatives (energy, number density) and second derivatives (specific heat, compressibility) for a one-component soliton gas (corresponding to the case of the low-temperature sine-Gordon chain). A complete description of the equilibrium statistical properties of the soliton gas is given in terms of the averages of occupation numbers and their *fluctuations*. The latter are characterized by the absence of off-diagonal correlations.

I. INTRODUCTION

The thermodynamics of soliton-bearing systems has attracted considerable attention since the fundamental observation[1] that topological solitons contribute an identifiable part to the free energy of the ϕ^4 chain. Integrable systems provide natural paradigms and illustrate the underlying structure that links the exact dynamics—in the form of phase-shift information and Hamiltonian formulation contained in inverse scattering theory (IST)—with Bethe-*Ansatz* (BA) thermodynamics.[2,3] The explicit link is provided by the soliton-gas phenomenology[4] which deals with solitons and nonlinear phonons as elementary excitations sharing the available phase space due to their phase-shift interactions.

The increasing degree of sophistication of the soliton picture[4–8] has revealed that it is in fact an exact scheme for reconstructing the thermodynamic free energy available by other means. Moreover, the soliton-gas scheme provides us "in passing" with a formidable amount of information regarding the microscopic distribution of the various nonlinear modes. Formally this information refers to occupation numbers and densities of available states in phase space. Whether these quantities are mere "bookkeeping" devices or actually possess a dynamical significance—detectable in, e.g., an inelastic neutron-scattering experiment–is not a settled question.

There is, however, another microscopic manifestation of the statistical properties of solitons: namely, their *fluctuations.* These may serve to characterize the degree of nonideality of the soliton gas and the ensuing deviations from Maxwell-Boltzmann statistics; they should show up in any direct reconstructions of thermodynamic second derivatives as well as in bona fide dynamical quantities, e.g., the soliton diffusion constant. We shall deal with the latter in a separate contribution, since the phenomenon itself is best illustrated in the context of numerical simulations. The theory of thermodynamic fluctuations can be handled analytically. It reveals an interesting mathematical property, namely, the absence of off-diagonal correlations between occupation numbers of different states. Although this property does not survive when we consider the phase-space densities—a natural consequence of the fact that we are dealing with an interacting system—it does suggest that there is something fundamental about occupation numbers and that, consequently, it would be sensible to keep the latter as distinct quantities in the theory.

The main point of this paper is to show that the fluctuations obtained about the most probable values of the occupation numbers possess the required degree of self-consistency within the framework of equilibrium statistical mechanics. In other words, it is possible to achieve a direct reconstruction of the relevant thermodynamic second derivatives. It may well be argued that this property by itself does not bestow our occupation numbers with any dynamical qualifications and that their status as bookkeeping devices remains untouched. However, the fact that it is possible to achieve a consistent description of thermodynamic fluctuations should be regarded as a further manifestation of the validity of the soliton-gas concept at a microscopic level. A more direct connection with the dynamics will be provided by the theory of soliton diffusion.

For the sake of notational simplicity we will present the theory for a single-component soliton gas. The most natural realization is the sine-Gordon (SG) breather gas, for which we will compute the relevant thermodynamic derivatives. Clearly the mathematical structure can be generalized in a straightforward manner. Furthermore, although we shall use a classical language and the corresponding Maxwell-Boltzmann expressions for the entropy, our statements remain valid for quantum mechanical systems solvable by the Bethe *Ansatz,* e.g., the one-dimensional δ-function Bose gas.

The paper is organized according to the order of thermodynamic derivative under discussion. Basic concepts and notation are presented along with the minimization of the thermodynamic potential in the following section (zeroth order). First derivatives (number densities, energy) are discussed in Sec. III. The theory of thermodynamic fluctuations is presented in Sec. IV, along with the direct reconstruction of the relevant second derivatives. Our conclusions are briefly summarized in Sec. V.

II. SOLITON STATISTICS

We consider a one-dimensional system of particles interacting via phase shifts. The exact statistical mechanics may be formulated by observing that the density of states (DOS) available to any given mode is reduced in the presence of other excited modes. Thus if $R_0(k)$ is the original DOS for the nonlinear mode characterized by k and $\Delta(k,k')$ the phase shift of mode k due to the presence of k', then the DOS $R(k)$ for the interacting system is given by

$$\frac{R(k)}{R_0(k)}=1-\frac{1}{L}\int dk'\Delta(k,k')R(k')n(k') , \tag{1}$$

where $n(k)$ is the occupation number of mode k, and L the length of the system. As indicated in the Introduction, we wish to maintain notational simplicity and therefore we restrict ourselves to one "species" of particles. In the context of the SG system this restricts us to low temperatures, as measured in units of the kink energy. This allows us to perform the analysis on the basis of an interacting breather gas. The symbol "k" stands for both parameters which describe the breather's state of motion, e.g., momentum and frequency of internal oscillation. The restriction to low temperatures can of course be removed by introducing a system of two coupled integral equations, as in the classical BA limit.[3] What is less clear is whether or not phonons have a legitimate position in the theory. Results for the Toda lattice suggest that they are essential. However, the current state-of-the-art calculations for the SG system[3,8] show clearly that the correct thermodynamics—available via the transfer-integral (TI) route—can be recovered using either (nonlinear) phonons or breathers. A similar result is obtained in the harmonic limit.[6] On the other hand, leading-order asymptotic expansions[5] allow *in principle* for breathers *and* phonons with the interesting result that the breather contribution vanishes. A similar conclusion can be reached in the harmonic limit,[9] where, conversely, phonons may be formally allowed, yet the minimization of the free energy forces the phonon DOS to vanish. In the absence of an exact solution of the full system of three coupled integral equations (two if kinks are neglected) we regard the issue as subtle and open. For the purpose of this work, where the emphasis lies on understanding fluctuations, it will be sufficient to consider a single-component (breather) soliton gas.

Equation (1) determines the amount of phase space available to all modes for any given configuration of occupation numbers $n(k)$. The actual number of solitons with parameters between k and $k+dk$ will be given by $\rho(k)dk$, where

$$\rho(k)=R(k)n(k) . \tag{2}$$

The following matrices will prove useful:

$$A(k,k')=-\frac{1}{L}R_0(k)n(k)\Delta(k,k') , \tag{3}$$

$$B(k,k')=\delta(k-k')+\frac{n(k)}{R(k')}\frac{\delta R(k)}{\delta n(k')} , \tag{4}$$

where $\delta R/\delta n$ denotes a functional derivative and

$$(\mathbf{1}-\mathbf{A})\cdot\mathbf{B}=\mathbf{1} \tag{5}$$

holds (cf. Ref. 7 and Appendix A). Multiplying (1) with $n(k)$ and using (5) we obtain

$$\rho(k)=\int dk' R_0(k')B(k,k')n(k') , \tag{6}$$

which provides the formal solution of (1) and will be of further use in what follows.

We consider a system of constant length and—for the time being—allow for a chemical potential μ to fix the number of particles. Bearing in mind that our "particles" are in fact excitations (breathers in our exemplary calculations), it is not *a priori* clear how we could physically control their total number, i.e., how the corresponding chemical potential could take any value different from zero. Topological excitations may couple to external "torques" which generate asymmetries between average numbers of kinks and antikinks. It is not obvious how one might "tune" the total number of nontopological solitons.

For any given configuration $n(k)$ the thermodynamic potential is given by

$$\Omega(\{n\})=\sum_k \hat{\Omega}(n_k)=\int dk\, R(k)\hat{\Omega}(n(k)) \tag{7}$$

with

$$\beta\hat{\Omega}(n(k))=n(k)\{\beta[E(k)-\mu]+\ln n(k)-1\} , \tag{8}$$

where $E(k)$ is the bare excitation energy and β the inverse temperature. At this stage it might be appropriate to remark that the only assumption entering (8) is that our excitations would obey Boltzmann statistics if phase shift interactions were turned off. Since we are dealing with a classical system this is in fact self-evident.

The minimization of Ω with respect to possible occupation numbers,

$$\left.\frac{\delta\Omega}{\delta n(k)}\right|_{\{n=\bar{n}\}}=0 , \tag{9}$$

yields the most probable occupation numbers,

$$\bar{n}(k)=e^{-\beta[\mathcal{E}(k)-\mu]} , \tag{10}$$

where $\mathcal{E}(k)$ is given by

$$\mathcal{E}(k)=E(k)+\frac{1}{\beta L}\int dk' R_0(k')\Delta(k',k)e^{-\beta[\mathcal{E}(k')-\mu]} \tag{11}$$

and the dependence of the renormalized energies on temperature and chemical potential has been suppressed for the sake of notational clarity. In the following, the over-bar for any quantity depending on the occupation configuration n will denote evaluation at $n=\bar{n}$.

Using the equilibrium values $\bar{n}(k)$ and the resulting equilibrium DOS $\bar{R}(k)$ results in the miraculously simple expression for the thermodynamic potential

$$-\beta\Omega=\int dk\,R_0(k)\bar{n}(k)\ , \tag{12}$$

where the bare DOS appears, so that a full description of thermodynamic properties is given by the equilibrium occupation numbers, i.e., by solving the integral equation (11). In the soliton context, Eq. (12) was first derived in Ref. 7, whereas (1) along with the minimization scheme were proposed in Ref. 10. The whole scheme is of course a transcription of the Yang and Yang-BA thermodynamics[11] for solitons rather than particles. Details of the derivation of (11) and (12) are given in Appendix B.

III. FIRST DERIVATIVES

We derive and briefly comment on the expressions for the total energy E, the number of excitations N and their detailed distributions. Using (10), (11), and (5) we obtain

$$\frac{\partial\bar{n}(k)}{\partial\mu}=\beta\bar{n}(k)\int dk'\bar{B}(k',k) \tag{13}$$

and

$$\frac{\partial\bar{n}(k)}{\partial\beta}=\bar{n}(k)\int dk'\bar{B}(k',k)[\mu-E(k')] \tag{14}$$

and hence

$$\begin{aligned}N=-\left[\frac{\partial\Omega}{\partial\mu}\right]_T&=\frac{1}{\beta}\int dk\,R_0(k)\frac{\partial\bar{n}(k)}{\partial\mu}\\&=\int dk\int dk'R_0(k)\bar{n}(k)\bar{B}(k',k)\\&=\int dk'\bar{\rho}(k')\ ,\end{aligned} \tag{15}$$

where we have made use of (6). The interpretation is obvious; we obtain excitations distributed according to the microscopic density (2). Differentiation of Ω with respect to μ yields the correct *total* number of excitations. However, it would be wrong to interpret the integrand in the first line of (15) as the microscopic number density $\bar{\rho}(k)$ in the interval dk [cf. Eq. (40) of Ref. 6], since the equality does not in general hold under the integral sign [cf. the derivation of the explicit form of $\rho(k)$ given at the end of this section for an exception]. In the next section we shall see that usage of the correct number density $\rho(k)$ or, alternatively, the DOS function $R(k)$ is essential for a consistent treatment of fluctuations and hence for construction of improved phenomenologies of dynamical correlation functions.

The total energy E can be obtained from the thermodynamic relation

$$E=\frac{\partial}{\partial\beta}(\beta\Omega)_{L,\mu}+\mu N=\int dk\,\rho(k)E(k)\ . \tag{16}$$

The last equation has the expected direct interpretation in terms of a *bare* energy multiplied by the correct density of excitations and integrated over all phase space. A similar equation, i.e., with bare masses (dilations/contractions) and the full densities (2), holds for the thermal expansion of the Toda lattice[9]—with separate contributions from the soliton and phonon sector, respectively.

The results presented so far in this section demonstrate that the exact reconstruction of thermodynamic first derivatives (Toda length, SG breather numbers and energies) demands knowledge of the phase-space density R in addition to the occupation numbers n. The formal solution (6) is however inadequate for practical purposes—as opposed to the formal manipulations leading to (11) and (12)—since it involves the generally intractable problem of inverting the matrix $(\mathbf{1}-\mathbf{A})$. At this stage it becomes vital to depart from our general procedure and exploit the *particular symmetries* of any given problem. In the SG case the Lorentz symmetry of the underlying wave equation implies

$$E(k)\Delta(k,k')=E(k')\Delta(k',k)\ .$$

If k stands for rapidity (and internal variable),

$$R_0(k')/R_0(k)=E(k')/E(k)$$

and thus

$$n(k')A(k,k')=n(k)A(k',k)\ , \tag{17}$$

$$n(k')B(k,k')=n(k)B(k',k)\ . \tag{18}$$

Using (6) and the above symmetry relationships we obtain

$$\begin{aligned}\frac{\bar{R}(k)}{R_0(k)}&=\int dk'\bar{B}(k,k')\frac{R_0(k')\bar{n}(k')}{R_0(k)\bar{n}(k)}\\&=\int dk'\frac{E(k')}{E(k)}\bar{B}(k',k)\\&=\frac{1}{E(k)}\frac{\partial}{\partial\beta}(\beta\epsilon(k))\end{aligned} \tag{19}$$

and

$$\bar{\rho}(k)=\bar{R}(k)\bar{n}(k)=-R_0(k)\frac{1}{E(k)}\frac{\partial}{\partial\beta}\bar{n}(k)\ , \tag{20}$$

where in the last step of (19) we have set $\mu=0$, appropriate to the case of the SG breather gas (cf. our discussion above). Using the expression (20) along with the analytical solution of Ref. 6 for $\bar{n}(k,\beta,\mu=0)$ we can verify that the total number of breathers (15) is equal to one-half the original (particle) degrees of freedom and that the energy (16) is indeed $1/\beta$ per particle, as expected in the harmonic limit of the SG chain. More interesting from our point of view is the explicit form of the DOS function

$$\frac{R}{R_0}=\coth\frac{\beta E(k)}{2}-\frac{2}{\beta E(k)}\ , \tag{21}$$

practically indistinguishable from the result obtained in the classical limit of the BA.[12] It is worth noting that the right-hand side (rhs) of (21) depends on the breather parameters only via the ratio of breather energy to temperature. For energies far above thermal levels, R/R_0 tends to unity; there is no restriction to the availability of phase-space—although of course such states have very low occupation probabilities $n(k)$. Conversely, for very low breather energies—where the occupation probability tends to unity—the available phase space, as measured by R/R_0, shrinks to zero.

In the case of the δ-function Bose gas[11] the relevant symmetry is $\Delta(k,k')=\Delta(k',k)$ and the bare density of states R_0 is a constant. Thus, although (17) and (18) are still valid, the first line of (19) now yields

$$\frac{\bar{R}(k)}{R_0}=\int dk'\bar{B}(k',k)=1-\frac{\partial}{\partial\mu}\epsilon(k) \tag{22}$$

and

$$\bar{\rho}(k)=R_0\frac{1}{\beta}\frac{\partial}{\partial\mu}\bar{n}(k) . \tag{23}$$

In this particular case the integrands in the first and last lines of (15) are identical.

IV. FLUCTUATIONS

In Sec. II we calculated thermodynamic averages by extremizing the thermodynamic potential Ω. The expressions (10) for average occupation numbers are such that they reduce to Boltzmann probabilities *when the phase shift interactions are turned off.* This of course does not imply Maxwell-Boltzmann statistics for our excitations, since any occupation number can in fact be brought into the form (10) if we are willing to accept thermally renormalized excitation energies $\mathcal{E}(k,T)$. The actual type of statistics involved in our system depends on the details of the phase shift functions and can ultimately be characterized by the behavior of the *fluctuations* of the occupation numbers around their equilibrium values.

The probability of occurrence of a fluctuation $\delta n(k)$ is controlled by

$$\begin{aligned}\beta[\Omega(\{\bar{n}+\delta n\})-\Omega(\{\bar{n}\})]=\tfrac{1}{2}\int dk\int dk'\,C(k,k')&\\ \times\delta n(k)\delta n(k')&\\ +O((\delta n)^3)\ ,&\end{aligned} \tag{24}$$

where $C(k,k')$ is the functional derivative of $\beta\Omega$ with respect to occupation numbers, taken at their equilibrium values:

$$\frac{1}{\beta}C(k,k')=\left.\frac{\delta^2\Omega(\{n\})}{\delta n(k)\,\delta n(k')}\right|_{\{n=\bar{n}\}} . \tag{25}$$

It is shown in Appendix C that the matrix $C(k,k')$ after a series of cancellations takes the diagonal form

$$C(k,k')=\frac{\bar{R}(k)}{\bar{n}(k)}\delta(k-k') , \tag{26}$$

which allows us to extract the Gaussian fluctuation averages

$$\langle\delta n(k)\delta n(k')\rangle=\frac{\bar{n}(k)}{\bar{R}(k)}\delta(k-k') . \tag{27}$$

The fact that there are no off-diagonal correlations in the n's indicates that there is a technical as well as a conceptual advantage in making a clear distinction between the *availability* of phase space and its thermal *occupation,* as expressed by the functions R and n, respectively. However, it does not allow us to draw the conclusion of complete statistical independence of modes belonging to different k's, since the physically important number densities $\rho(k)$ exhibit fluctuations according to

$$\langle\delta\rho(k)\delta\rho(k')\rangle=\int dk''\bar{\rho}(k'')\bar{B}(k,k'')\bar{B}(k',k'') , \tag{28}$$

i.e., contain in general an off-diagonal contribution.

Equation (28) is obtained by making use of

$$\frac{\delta\rho(k)}{\delta n(k')}=B(k,k')R(k') , \tag{29}$$

which in turn follows directly from the definition of $\rho(k)$ and (4).

We may now proceed to test the consistency of the fluctuation formulas by performing a direct calculation of $\langle(\delta N)^2\rangle$ and $\langle(\delta E)^2\rangle$ and comparing with the corresponding thermodynamic derivatives. It will be helpful to use the auxiliary relationships

$$\frac{\partial\rho(k)}{\partial\beta}=\int dk'R(k')B(k,k')\frac{\partial n(k')}{\partial\beta} , \tag{30}$$

$$\frac{\partial\rho(k)}{\partial\mu}=\int dk'R(k')B(k,k')\frac{\partial n(k')}{\partial\mu} , \tag{31}$$

both derivable from (29). Using (15) we find

$$\delta N=\int dk\,\delta\rho(k) \tag{32}$$

and

$$\langle(\delta N)^2\rangle=\int dk\int dk'\int dk''\bar{\rho}(k'')\bar{B}(k,k'')\bar{B}(k',k'') \tag{33}$$

in agreement with the thermodynamic derivative

$$\langle(\delta N)^2\rangle=\frac{1}{\beta}\left[\frac{\partial N}{\partial\mu}\right]_T , \tag{34}$$

obtainable by direct differentiation of (15) and application of (31).

Energy fluctuations can be similarly computed using

$$\delta E=\int dk\,E(k)\delta\rho(k) \tag{35}$$

$$\begin{aligned}\langle(\delta E)^2\rangle=\int dk\int dk'\int dk''\bar{\rho}(k'')E(k)E(k')&\\ \times\bar{B}(k,k'')\bar{B}(k',k'') ,&\end{aligned} \tag{36}$$

in agreement with the result obtained via the thermodynamic derivative

$$\langle(\delta E)^2\rangle=\frac{1}{\beta^2}C_L=-\frac{\partial^2}{\partial\beta^2}(\beta\Omega) , \tag{37}$$

where we have taken $\mu=0$ in the last equation.

Equations (32)–(37) demonstrate that our treatment of fluctuations does indeed pass the self-consistency test, in the sense that fluctuation averages calculated within the spirit of soliton phenomenology[4] are in exact agreement with the results obtained from thermodynamic derivatives. Using (27) and (28) averages of arbitrary fluctuating quantities can be computed in the Gaussian approximation. Thus Eqs. (27) and (28) provide us with a complete formal description of soliton statistics. In addition, the rhs of (27) suggests a direct physical interpretation: (classical) solitons exhibit Boltzmann-type fluctuation properties, except for an overall phase-space restriction factor $\bar{R}/R_0$ in the denominator. Since $\bar{R}$ is a functional of all $\bar{n}(k)$ this may be technically quite nontrivial (note, however, that our use of explicit symmetry properties may facilitate even this technical aspect). Yet the physical content seems rather straightforward. Indeed this is the sort of relationship one might have conjectured in the context of an *ad hoc* treatment of soliton statistics. The fact that it can be *proved* is certainly gratifying and should lend further credibility to dynamical phenomenologies which have to rely on a correct description of equilibrium statistical properties.[13,14]

V. CONCLUDING REMARKS

We have presented a treatment of the statistical properties of solitons in integrable systems. The picture which arises in the SG context—and can readily be generalized to other systems—can be summarized as follows: Solitons are distributed in phase space according to the density of states $R(k)$ available in the neighborhood of a particular point and according to an occupation number $n(k)$ specifying the probability of occupation of a given available state. The equilibrium values of $n(k)$ and $R(k)$ can be obtained by minimization of the appropriate thermodynamic potential. Furthermore, the fluctuations of the n's around their equilibrium values can be calculated exactly and are characterized by the absence of off-diagonal correlations.

For classical systems it is thus possible to maintain the fiction of Boltzmann statistics (in spite of the interacting nature of our system), provided we are willing to incorporate into our formalism (i) thermally renormalized soliton energies and (ii) the overall phase-space restrictions which determine the density of actually available states and the behavior of thermal fluctuations. Alternatively, we may regard the thermal averages $\bar{n}(k)$ and the fluctuations $\langle[\delta n(k)]^2\rangle$ as "carriers" of information regarding the exact nature of the solitons' statistical properties.

The thermodynamic properties of soliton-bearing systems can be exactly reconstructed on the basis of what has commonly been referred to as soliton phenomenology. The high degree of self-consistency manifested in the agreement of fluctuation averages with the corresponding thermodynamic derivatives and the absence of off-diagonal correlations support the validity and the usefulness of "direct" soliton statistics.

APPENDIX A

Functional differentiation of both sides of (1) with respect to $\delta n(k')$ leads to

$$\frac{1}{R_0(k)}\frac{\delta R(k)}{\delta n(k')}=-\frac{1}{L}\int dk''\Delta(k,k'')\left[R(k'')\delta(k'-k'')+n(k'')\frac{\delta R(k'')}{\delta n(k')}\right]. \tag{A1}$$

Multiplying by $n(k)R_0(k)/R(k')$ and using the definition of $\mathbf{A}$, Eq. (3), we obtain

$$\frac{n(k)}{R(k')}\frac{\delta R(k)}{\delta n(k')}=\int dk''A(k,k'')\times\left[\delta(k'-k'')+\frac{n(k'')}{R(k')}\frac{\delta R(k'')}{\delta n(k')}\right], \tag{A2}$$

or, inserting (4),

$$B(k,k')-\delta(k-k')=\int dk''A(k,k'')B(k'',k'), \tag{A3}$$

which can be written in compact form as

$$\mathbf{B}-\mathbf{1}=\mathbf{A}\cdot\mathbf{B}. \tag{A4}$$

APPENDIX B

Functional differentiation of the thermodynamic potential with respect to $n(k)$ yields

$$\frac{\delta(\beta\Omega)}{\delta n(k)}=R(k)\{\beta[E(k)-\mu]+\ln n(k)\}+\int dk'\frac{\delta R(k')}{\delta n(k)}n(k')\{\beta[E(k')-\mu]+\ln n(k')-1\}. \tag{B1}$$

At the extremum demanded by (9),

$$\beta[E(k)-\mathcal{E}(k)]+\int dk'[\bar{B}(k',k)-\delta(k'-k)]\{\beta[E(k')-\mathcal{E}(k')]-1\}=0, \tag{B2}$$

where the overbars denote that $n(k)=\bar{n}(k)=\exp\{-\beta[\mathcal{E}(k)-\mu]\}$. We now rewrite (B2) as

$$\int dk'\bar{B}(k',k'')\beta[\mathcal{E}(k')-E(k')]=1-\int dk'\bar{B}(k',k'')=\int dk'[\delta(k'-k'')-\bar{B}(k',k'')], \tag{B3}$$

multiply both sides of (B3) by $[\delta(k''-k)-\bar{A}(k'',k)]$ and integrate over dk'', obtaining

$$\beta[\mathcal{E}(k)-E(k)]=-\int dk'\bar{A}(k',k)=\frac{1}{L}\int dk'R_0(k')\Delta(k',k)e^{-\beta[\mathcal{E}(k)-\mu]}, \tag{B4}$$

i.e., the integral equation (11) determining the thermally renormalized soliton energies $\{\mathcal{E}(k)\}$ in terms of the phase shifts $\{\Delta(k,k')\}$. The expressions for the thermodynamic potential (12) follow trivially by using (B4) and (5) in

$$\beta\Omega=\beta\Omega(\{\bar{n}(k)\})=-\int dk'\bar{R}(k')\bar{n}(k')\{1+\beta[\mathcal{E}(k')-E(k')]\}\ , \tag{B5}$$

or

$$-\beta\Omega=\int dk'\int dk''\int dk\bar{R}_0(k'')\bar{n}(k'')\bar{B}(k',k'')[\delta(k-k')-\bar{A}(k,k')]=\int dk\, R_0(k)\bar{n}(k)\ . \tag{B6}$$

APPENDIX C

The fundamental second derivative (24) can be obtained by a further functional differentiation of (B1):

$$\begin{aligned}\frac{\delta^2(\beta\Omega)}{\delta n(k)\delta n(k')}=&\frac{\delta R(k)}{\delta n(k')}\{\beta[E(k)-\mu]+\ln n(k)\}\\&+\frac{R(k)}{n(k)}\delta(k-k')+\frac{\delta R(k')}{\delta n(k)}\{\beta[E(k')-\mu]+\ln n(k')-1+1\}\\&+\int dk''\frac{\delta^2 R(k'')}{\delta n(k)n(k')}n(k'')\{\beta[E(k'')-\mu]+\ln n(k'')-1\}\ ,\end{aligned} \tag{C1}$$

or, at equilibrium $\{n=\bar{n}\}$,

$$\begin{aligned}C(k,k')=&[\bar{B}(k,k')-\delta(k-k')]\frac{\bar{R}(k')}{\bar{n}(k)}\beta[E(k)-\mathcal{E}(k)]+k\leftrightarrow k'+\frac{\bar{R}(k)}{\bar{n}(k)}\delta(k-k')\\&-\int dk''\frac{\delta^2 R(k'')}{\delta n(k)n(k')}\bigg|_{\{n=\bar{n}\}}\bar{n}(k'')\{1+\beta[\mathcal{E}(k'')-E(k'')]\}\ .\end{aligned} \tag{C2}$$

The rhs of (C2) contains a contribution diagonal in k,k' [the third term (III)], and other explicitly symmetric contributions, e.g., the sum of first and second terms (I + II) or the fourth term (IV). Of those, only (IV) contains the unknown second derivative $\delta^2 R/\delta n\,\delta n$, which we proceed to compute. From (A1) we obtain

$$\frac{\delta R(k)}{\delta n(k')}=-\frac{1}{L}R_0(k)\Delta(k,k')R(k')-\frac{1}{L}\int d\bar{k}\, R_0(k)\Delta(k,\bar{k})\frac{\delta R(\bar{k})}{\delta n(k')}n(\bar{k}) \tag{C3}$$

and

$$\begin{aligned}\frac{\delta^2 R(k)}{\delta n(k')\delta n(k'')}=&-\frac{1}{L}R_0(k)\Delta(k,k')\frac{\delta R(k')}{\delta n(k'')}-\frac{1}{L}R_0(k)\Delta(k,k'')\frac{\delta R(k'')}{\delta n(k')}\\&-\frac{1}{L}\int d\bar{k}\, R_0(k)\Delta(k,\bar{k})\frac{\delta^2 R(\bar{k})}{\delta n(k')\delta n(k'')}n(\bar{k})\ .\end{aligned} \tag{C4}$$

Defining

$$\chi(k;k',k'')=n(k)\frac{\delta^2 R(k)}{\delta n(k')\delta n(k'')} \tag{C5}$$

we readily obtain

$$\begin{aligned}\int d\bar{k}[\delta(k-\bar{k})-A(k,\bar{k})]\chi(\bar{k};k',k'')=&A(k,k')[B(k',k'')-\delta(k'-k'')]\frac{R(k'')}{n(k')}\\&+A(k,k'')[B(k'',k')-\delta(k''-k')]\frac{R(k')}{n(k'')}\ ,\end{aligned} \tag{C6}$$

or, using the fact that $\mathbf{B}\cdot(\mathbf{1}-\mathbf{A})=\mathbf{1}$,

$$\begin{aligned}\chi(k'';k,k')=&[B(k'',k)-\delta(k''-k)][B(k,k')-\delta(k-k')]\frac{R(k')}{n(k)}\\&+[B(k'',k')-\delta(k''-k')][B(k',k)-\delta(k'-k)]\frac{R(k)}{n(k')}\ .\end{aligned} \tag{C7}$$

With the help of (C7) we proceed to evaluate term IV in (C2), i.e.,

$$-\int dk''\bar{\chi}(k'';k,k')\{1+\beta[\mathcal{E}(k'')-E(k'')]\}\ . \tag{C8}$$

Since the two terms in the rhs of (C7) only serve to guarantee the symmetry of $\chi(k'';k,k')$ under the interchange of k,k' we only need to compute the contribution of the first term. The first factor enclosed in square brackets is the only quantity dependent on k'' and thus entering under the integral (C8). Now

$$\begin{aligned}-\int dk''[\bar{B}(k'',k)-\delta(k''-k)]\{1+\beta[\mathcal{E}(k'')-E(k'')]\}&=1+\beta[\mathcal{E}(k)-E(k)]-1\\&=\beta[\mathcal{E}(k)-E(k)]\end{aligned} \tag{C9}$$

generates a contribution to (C8),

$$\beta[\mathcal{E}(k)-E(k)][\bar{B}(k,k')-\delta(k-k')]\frac{\bar{R}(k')}{\bar{n}(k')}\ ,$$

which cancels the first term in (C2). Similarly the second term in (C7) generated by the interchange $k\leftrightarrow k'$ cancels the second term in (C2) leaving us with (III),

$$C(k,k')=\frac{\bar{R}(k)}{\bar{n}(k)}\delta(k-k')\ . \tag{C10}$$

---

*Permanent address: Fakultät für Physik, Universität Konstanz, D-7750 Konstanz, FRG.

[1] J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B **11**, 3535 (1974).
[2] N. Theodorakopoulos, Phys. Rev. Lett. **53**, 871 (1984); M. Opper, Phys. Lett. **112A**, 201 (1985).
[3] N.-N. Chen, M. D. Johnson, and M. Fowler, Phys. Rev. Lett. **56**, 904 (1986); M. D. Johnson, N.-N. Chen, and M. Fowler, Phys. Rev. B **34**, 7851 (1986).
[4] J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger, Phys. Rev. B **22**, 477 (1980).
[5] N. Theodorakopoulos, Z. Phys. B **46**, 367 (1982) and Phys. Rev. B **30**, 4071 (1984).
[6] K. Sasaki, Phys. Rev. B **33**, 2214 (1986).
[7] H. Takayama and M. Ishikawa, Prog. Theor. Phys. **74**, 479 (1985).
[8] J. Timonen, M. Stirland, D. J. Pilling, Yi Cheng, and R. K. Bullough, Phys. Rev. Lett. **56**, 2233 (1986).
[9] N. Theodorakopoulos (unpublished).
[10] N. Theodorakopoulos, in *Dynamical Problems in Soliton Physics*, edited by S. Takeno (Springer, Berlin, 1985), p. 115.
[11] C. N. Yang and C. P. Yang, J. Math. Phys. **10**, 1115 (1969).
[12] M. Fowler, Phys. Rev. B **26**, 2514 (1982).
[13] K. Maki and K. Sasaki, Phys. Rev. B **35**, 257 (1987); **35**, 263 (1987).
[14] N. Theodorakopoulos and E. W. Weller (unpublished).