Classical Thermodynamics of the Toda Lattice

— As a Classical Limit of the Two-Component Bethe Ansatz Scheme —

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In our previous work thermodynamics of two-component (soliton and phonon) gas is constructed from the Yang-Yang equation for one-component integrable quantum gas. We call this the two-component Bethe ansatz (TCBA) scheme. The method is applied to the Toda lattice and its classical limit is analyzed. The key parameter $\kappa^2$ which distinguishes solitons from phonons within the TCBA scheme is chosen such that the resultant equations for effective energies of the modes coincide with those expected from the simple-minded ideal-gas phenomenology. The soliton specific heat exhibits a peculiar temperature dependence at low temperatures. It is however compensated with the anharmonic part of phonons.

§ 1. Introduction

The statistical mechanics of one-dimensional soliton-bearing systems has been extensively studied in this decade. A major interest in such a study is to clarify the role of solitons in thermodynamics of the systems. Among the latter the Toda lattice is a typical example. Its classical Hamiltonian is known to be separable into the soliton and phonon (or ripple) modes and completely integrable,\(^1\) while its classical thermodynamic potential can be exactly evaluated.\(^2\) The latter, however, does not separate the roles of solitons and phonons in thermodynamics. Inspired by the pioneering work by Krumhansl and Schrieffer\(^3\) several researchers have discussed the two-component ideal-gas phenomenology also on the Toda lattice.\(^4\)\(-7\)

A breakthrough of the problem has been realized by means of the Bethe ansatz (BA) method, particularly, by the Yang-Yang (YY) theory\(^8\) on the quantum statistical mechanics of integrable systems. The method has been first applied to the sine-Gordon system and successfully separated the role of solitons in thermodynamics.\(^9\)\(^,\)\(^10\) In our previous work\(^1\)\(^1\) (hereafter referred to as I) we have discussed a close relationship between the BA approach and an extended ideal-gas phenomenological (EIGP) approach. The latter is an ideal-gas model, in which, however, the interactions between the modes yielding phase-shifts for phonons, or spatial displacements for solitons are self-consistently taken into account.

As for the Toda lattice the BA scheme itself was first questioned since the interaction potential is not of a $\delta$-function type. However as far as the quantities described by the phase-shifts of interacting particles are concerned, its validity has been proved in a way that it reproduces the proper dispersion of the soliton and phonon excitations in the classical limit.\(^12\)\(^,\)\(^13\) This analysis has been extended to finite temperatures for the quantum Toda lattice.\(^14\) The classical version of the YY equation has been first obtained and numerically analyzed by Theodorakopoulos.\(^15\) Later his equation has been exactly solved by Opper,\(^16\) thereby Toda’s exact thermodynamic potential\(^17\) has been reproduced. However in the latter work, as in Toda’s, the roles of solitons and phonons are not
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The aim of the present work is to investigate this last problem, i.e., to clarify the roles of solitons and phonons in the classical thermodynamics of the Toda lattice. For this purpose we adopt our previous analysis in I, by which the YY theory is rewritten as thermodynamics of two-component (phonon-soliton) gas system. Here we call it the two-component Bethe ansatz (TCBA) scheme. In the original YY equation the variable is the momentum \( k \) of the original quantum particles. A two-component gas model is constructed by separating the \( k \)-space into two, namely \(|k|\leq k_F\) and \(|k|>k_F\). The key parameter \( k_F \) of the separation is well-defined at zero temperature. It directly specifies the (quantum) ground state of the original system, and the excitations associated with the \(|k|\leq k_F(>k_F)\) branch are ascertained as phonons (solitons).\(^{12,13}\) The problem is then whether we can specify such a \( k_F \) at finite temperatures and in the classical limit. Hader and Mertens\(^{14}\) have proposed one way to specify \( k_F \) in the quantum Toda lattice, while in the classical limit Theodorakopoulos\(^{15}\) has proposed a different definition of \( k_F \) by solving his equation numerically. We propose in this work another specification of \( k_F \) by comparing the TCBA scheme with a simple-minded EIGP scheme for the classical thermodynamics.

Interestingly the TCBA scheme is formally constructed from the YY theory without specifying an explicit value for \( k_F \), although in I we adopted the value at zero temperature. Furthermore the phase-shift functions (which represent effects of the pairwise interactions between modes) of the Toda lattice are explicitly solved in the classical limit, and are shown to coincide exactly with those derived from the classical inverse scattering method.\(^{17}\) The resulting coupled equations, which determine effective phonon and soliton energies, are essentially identical to Theodorakopoulos’ equation,\(^{15}\) in which the separation of the \( k \)-space is not introduced. Then we specify the value \( k_F \) such that the resultant equations coincide with those expected from the EIGP scheme.

Having specified \( k_F \), we can evaluate separately the contributions of solitons and phonons to, for example, the Gibbs free energy. Their asymptotic expressions at low temperatures are hardly obtained as already pointed out by Theodorakopoulos.\(^{15}\) Numerical analysis reveals a peak in the soliton specific heat (under fixed pressure) at low temperatures (see Fig. 3 below). It is, however, compensated by the anharmonic phonon contributions. The total specific heat exhibits only a simple power-law dependence on temperature, which is Toda’s result.\(^2\) In this sense it seems difficult to observe soliton effects separately in thermodynamic quantities. We believe, however, that the present analysis specifies most naturally phonons and solitons, and gives correctly their populations at finite temperatures.

This paper is arranged as follows: In § 2 we review general derivation of the TCBA scheme from the YY theory, emphasizing the fact that we need not specify the value of the key parameter \( k_F \). This TCBA scheme is applied to the Toda lattice, and is solved in the classical limit in § 3. There the relation of our TCBA scheme with Theodorakopoulos’ equation and Oppen’s solution is also pointed out. Summary and discussion on the results are given in the last section.

§ 2. Derivation of the two-component Bethe ansatz (TCBA) scheme

We consider an integrable quantum system whose Hamiltonian is given by
\[ H = \sum_{n=1}^{N} \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_n^2} + \sum_{m>n} V(x_n - x_m) \right\}. \]  

(2.1)

Following the Yang-Yang theory, after an appropriate scaling of the length and energy thermodynamic quantities of the system can be written down in terms of the density distributions of 'particles' and 'holes' with the momentum \( k\), \( \rho(k) \) and \( \rho_h(k) \), respectively. The particle density \( d \), for example, is given by

\[ d = \frac{N}{L} \int_{-\infty}^{\infty} dk \rho(k). \]  

(2.2)

The distributions \( \rho(k) \) and \( \rho_h(k) \) obey the following condition:

\[ \frac{1}{2\pi} = \rho(k) + \rho_h(k) + \int_{-\infty}^{\infty} dk' T(k-k') \rho(k'), \]  

(2.3)

where \( T(k) \equiv (2\pi)^{-1} d\theta/dk, \theta(k) \) being the phase-shift of the particles due to mutual interactions. The minimization of the free energy with respect to \( \rho(k) \) and \( \rho_h(k) \) under the constraints (2.2) and (2.3) yields the YY equation

\[ \epsilon(k) = \frac{1}{\beta} \ln \frac{\rho_h(k)}{\rho(k)} = k^2 - \mu + \frac{1}{\beta} \int_{-\infty}^{\infty} dk' T(k-k') \ln(1 + e^{-\beta\epsilon(k')}), \]  

(2.4)

where \( \beta = 1/T \) (\( k_B = 1 \)) and \( \mu \) is the chemical potential. The equilibrium free energy \( F \) and the pressure \( p \) are given by

\[ f = \frac{F}{L} = -A + \mu d, \]  

(2.5)

\[ p = -\left( \frac{\partial F}{\partial L} \right)_T = A, \]  

(2.6)

where

\[ A = \frac{1}{2\pi\beta} \int_{-\infty}^{\infty} dk \ln(1 + e^{-\beta\epsilon(k)}). \]  

(2.7)

Now we construct a two-component gas model by dividing the \( k \)-space into the two: \( |k| \leq k_F \) and \( |k| > k_F \). In contrast to our previous work I, we do not specify at the moment any physical meaning on \( k_F \) and so its explicit value, and develop an entirely formal argument. As in we use the notations \( k_1 \) and \( k_2 \) such that \( |k_1| \leq k_F \) and \( |k_2| > k_F \), and the abbreviations \( \int_{|k| \leq k_F} dk \cdots = \int_{dk(1)} \cdots \).

By means of the phase-shift functions \( K_{ij}(k_1, k_2) \) defined by

\[ K_{11}(k_1, k_1') = \delta(k_1 - k_1') - \int dk'' T(k_1 - k''') K_{11}(k_1'', k_1'), \]  

(2.8a)

\[ K_{12}(k_1, k_2) = -\int dk' T(k_2 - k_1') K_{11}(k_1', k_1) = K_{21}(k_2, k_1), \]  

(2.8b)

\[ K_{22}(k_2, k_2') = -\delta(k_2 - k_2') - T(k_2 - k_1') - \int dk_1 T(k_2 - k_1) K_{12}(k_1, k_2'), \]  

(2.8c)

where \( \delta(k) \) is the delta function, Eq. (2.3) is reduced to
\[
\begin{align*}
\rho(k_1) &= \rho^b(k_1) - \int dk_1' K_{11}(k_1, k_1') \rho_n(k_1') + \int dk_2 K_{12}(k_1, k_2) \rho(k_2), & (2.9a) \\
\rho_n(k_2) &= \rho_n^b(k_2) - \int dk_1 K_{21}(k_2, k_1) \rho_n(k_1) + \int dk_2' K_{22}(k_2, k_2') \rho(k_2'), & (2.9b)
\end{align*}
\]

where
\[
\begin{align*}
\rho^b(k_1) &= \frac{1}{2\pi} \int dk_1' K_{11}(k_1, k_1'), & (2.10a) \\
\rho_n^b(k_2) &= \frac{1}{2\pi} \left\{ 1 + \int dk_1 K_{21}(k_2, k_1) \right\}. & (2.10b)
\end{align*}
\]

Similarly Eq. (2.4) becomes coupled equations for \(\varepsilon(k_1)\) and \(\varepsilon(k_2)\), which are rewritten as the following equations for \(E_1(k_1)\) and \(E_2(k_2)\) defined by
\[
\exp[\pm \beta \varepsilon(k_i)] = \{ \exp[\beta E_i(k_i)] - 1 \}^{-1},
\]

where the signature \(+(-)\) is for \(i = 1(2),\)
\[
\begin{align*}
E_1(k_1) &= e_1(k_1) + \int dk_1' K_{11}(k_1, k_1') f_1(k_1') - \int dk_2 K_{12}(k_1, k_2) f_2(k_2), & (2.12a) \\
E_2(k_2) &= e_2(k_2) - \int dk_1 K_{21}(k_2, k_1) f_1(k_1) + \int dk_2' K_{22}(k_2, k_2') f_2(k_2'), & (2.12b)
\end{align*}
\]

where
\[
\begin{align*}
e_1(k_1) &= \int dk_1' K_{11}(k_1, k_1') (\mu - k_1'^2), & (2.13a) \\
e_2(k_2) &= k_2^2 - \mu + \int dk_1 K_{21}(k_2, k_1) (k_1^2 - \mu) & (2.13b)
\end{align*}
\]

and
\[
f_i(k_i) = -\beta^{-1} \ln \{ 1 - \exp[-\beta E_i(k_i)] \}. & (2.14)
\]

In terms of \(f_i(k_i)\) the constant \(A\) defined by Eq. (2.7) is written as
\[
A = \frac{1}{2\pi} \int dk_1 e_1(k_1) - \int dk_1 \rho^b(k_1) f_1(k_1) - \int dk_2 \rho_n^b(k_2) f_2(k_2). & (2.15)
\]

The above equations are interpreted as follows. The system consists of two components of gas specified by \(k_i\) \((i = 1 \text{ and } 2)\). Their bare excitation energies and bare densities of states are \(e_1(k_1)\) and \(e_2(k_2)\), and \(\rho^b(k_1)\) and \(\rho_n^b(k_2)\), respectively. They are modified due to the mutual interaction whose effects are described by \(K_{ij}(k_i, k_j)\), instead of \(T(k - k')\). The final expression of the free energy (Eq. (2.5) combined with Eq. (2.15)) tells, however, that the system can be still regarded as a two-component ideal gas. One only needs to use the modified excitation energy \(E_i(k_i)\) in the expression of the free energy of each component, \(f_i\) of Eq. (2.14).

On the other hand, the simple-minded EIGP scheme is as follows. Suppose the classical Hamiltonian of an integrable system is separable into two modes with the dispersion relation \(e_i(p_i), i = 1, 2\). Among the modes there exist pair-wise elastic interactions, by which each mode suffers from phase-shift (phonon) or spatial displacement
(soliton). The latter gives rise to the change of the density of states of the modes. Let
this change of the $i$-th mode with momentum $p_i$ due to the presence of the $j$-th mode with
momentum $p_j$ be $\Delta_{ij}(p_i, p_j)$, which can be evaluated in principle by the classical inverse
scattering method. If the effects of this change are taken into account self-consistently,
and if the vanishing chemical potential and the Bose statistics are assumed for each mode,
then it is shown in I that the total free energy $f$ is given by

$$ f = \frac{2}{\pi} \int \frac{dp_i}{2\pi} f_i^{(0)}(p_i), \quad (2.16) $$

where

$$ f_i^{(0)}(p_i) = -\frac{1}{\beta} \ln \{ 1 + n_i(p_i) \}, \quad (2.17) $$

$$ n_i(p_i) = \{ \exp[\beta E_i(p_i)] - 1 \}^{-1}. \quad (2.18) $$

and the effective energies $E_i(p_i)$ are determined by

$$ E_i(p_i) = e_i(p_i) + \frac{\sum_{j=1}^{2} \int dp_j \Delta_{ij}(p_i, p_j) f_j^{(0)}(p_j)}{2 \pi}, \quad (2.19) $$

for $i = 1, 2$. The densities of states $R_i(p_i)$ are given by solving the following equations:

$$ R_i(p_i) = \frac{1}{2 \pi} + \frac{\sum_{j=1}^{2} \int dp_j \Delta_{ij}(p_i, p_j) n_j(p_j)}{\pi}, \quad (2.20) $$

for $i = 1, 2$. One can at once notice the correspondences of Eqs. (2.16) with (2.5) combined
with (2.15), (2.17) with (2.14), (2.18) with (2.11), (2.19) with (2.12), and (2.20) with (2.9) (or more explicitly (3.11) below).

In the next section we will apply the above TCBA scheme to the Toda lattice, and
solve it explicitly in the classical limit. Here we emphasize again that only Eq. (2.8) has
been used without any specification of $k_F$ at all in the above arguments. An explicit value
for $k_F$ will be determined in the next section, thereby the correspondence between the two
approaches mentioned above will be also made much clearer.

### § 3. Classical Thermodynamics of the Toda Lattice

#### 3.1. Model

For the Toda lattice the potential $V(r)$ in Eq. (2.1) is specified by

$$ V(r) = \frac{m \omega^2}{\gamma^2} \left[ e^{-r(r-r_0)} + \gamma (r-r_0) \right]. \quad (3.1) $$

Following Mertens\(^{13}\) we scale all lengths by $1/\gamma$ and energies by $\hbar^2 \gamma^2 / 2m$ (the energy thus
scaled is indicated by the bar), and obtain

$$ \bar{H} = \sum_{n=1}^{N} \left\{ -\frac{\partial^2}{\partial x_n^2} + 2 C^2 \exp[-(x_{n+1} - x_n - r_0)] + V_0 \right\}, \quad (3.2) $$

where $C = m \omega / \hbar \gamma$ is the ratio of the characteristic energy of soliton $E_s = m \omega^2 / \gamma^2$ to that
of phonon $\hbar \omega$, and only this parameter involves the Planck constant $\hbar$. The constant
term $V_0$ is given by $V_0 = 2C^3(a - r_0)$ where $a = 1/d$ is the lattice constant; namely, we will solve thermodynamics by means of the YY theory under the constraint of a given lattice distance, or a particle density (Eq. (2.2)). Note that $a$ is not necessarily equal to $r_0$, at which $V(r)$ is minimum ($x_n$ in Eq. (3.2) is the coordinate, not the relative displacement from the equi-distance lattice points, of the $n$-th particle). This discrepancy is due to the pressure or/and thermal expansion effects.

Mathematically most of the equations in §2 hold true except for slight modifications due to the linear part of the Toda potential in Eq. (3.1). The term $2C^2$ has to be added and subtracted from Eqs. (2.5) and (2.6), respectively, and $\tilde{\mu}$ except for in Eq. (2.5) has to be replaced by $\tilde{\mu} + 2C^2r_0 = \tilde{\mu}$. In the classical limit $\hbar \to 0$ or $C \to \infty$, the derivative of the phase-shift $T(k)$ due to the Toda potential is given by

$$T(k) = \frac{1}{2\pi} \left( r_0 - 22 \ln \frac{|k|}{C} \right) = \frac{1}{2\pi} \left( \tilde{r}_0 - 2 \ln |\tilde{k}| \right),$$

(3.3)

where $\tilde{k} = k/k_F$ and

$$\tilde{r}_0 = r_0 - 2 \ln \frac{k_F}{C} = r_0 - 2 \ln \tilde{k}_F.$$

(3.4)

Here $k_F = \tilde{k}_F C$ is assumed of the order of $C$ without specifying the value of $\tilde{k}_F$ ($\sim O(\hbar^0)$) yet. But we of course expect that the modes with $|k| \leq k_F (> k_F)$ correspond to phonons (solitons) as in the $T = 0$ case.

3.2. Solution of $K_{\epsilon_3}(k_1, k_1')$

In terms of the scaled momenta $\tilde{k}_1$, where $|\tilde{k}_1| \leq 1$ and $|\tilde{k}_2| > 1$, Eq. (2.8a) is written as

$$K_{11}(k_1, k_1') = \frac{1}{k_F} \delta(\tilde{k}_1 - \tilde{k}_1') - k_F \int d\tilde{k}_1'' T(\tilde{k}_1'' - \tilde{k}_1') K_{11}(k_1'', k_1').$$

(3.5)

One can immediately see that $K_{11}$ on the l.h.s. of Eq. (3.5) is negligible in the classical limit ($k_F \to \infty$), and one only needs to solve for $\tilde{k}_1 \neq \tilde{k}_1'$

$$\int d\tilde{k}_1'' T(\tilde{k}_1'' - \tilde{k}_1') K_{11}(k_1'', k_1') = 0.$$  

(3.5')

Its solution is given by

$$K_{11}(k_1, k_1') = k_F^{-2} \left\{ K_{11}(\tilde{k}_1, \tilde{k}_1') \gamma K_{11}(\tilde{\gamma}_{11}, k_1', \tilde{k}_1') \right\},$$

(3.6)

where

$$K_{11}(\tilde{k}_1, \tilde{k}_1') = \frac{1}{\pi \delta_{1}(\tilde{k}_1)} \frac{\partial}{\partial \tilde{k}_1'} \left( s_{1}(\tilde{k}_1') \right),$$

(3.6a)

$$K_{11}(\tilde{k}_1, \tilde{k}_1') = 2 / \left\{ \pi \delta_{1}(\tilde{k}_1) s_{1}(\tilde{k}_1') \right\},$$

(3.6b)

with $s_{1}(\tilde{k}_1) \equiv (1 - \tilde{k}_1^2)^{1/2}$ and

$$\gamma = \tilde{r}_0 + 2 \ln 2.$$  

(3.7)

*) Another caution is on the singularity at $\tilde{k}_1 = \tilde{k}_1'$ in Eq. (3.6a). Equation (3.6) is the solution of Eq. (3.5') if the singular contribution from $\tilde{k}_1 \approx \tilde{k}_1'$ is discarded.
The overall constant of $K_{12}(k_1, k_1')$ cannot be determined by Eq. (3.5') alone. Its value is chosen here such that the resulting $K_{12}^{(0)}(\vec{k}_1, \vec{k}_2)$ correspond properly to those derived from the analyses based on the classical inverse scattering as we will discuss below (see the footnote below Eq. (3.16)). Substituting Eq. (3.6) into Eq. (2.8b) and then Eq. (2.8c), we obtain

$$K_{12}(k_1, k_2) = k_F^{-1}\{K_{12}^{(0)}(\vec{k}_1, \vec{k}_2) + \frac{1}{r}K_{12}^{(1)}(\vec{k}_1, \vec{k}_2)\}, \quad (3.8)$$

$$K_{12}^{(0)}(\vec{k}_1, \vec{k}_2) = -\frac{\text{sgn}(\vec{k}_2)}{\pi\langle k_2 \rangle k_1} \frac{s_2(\vec{k}_2)}{s_1(\vec{k}_1)}, \quad (3.8a)$$

$$K_{12}^{(1)}(\vec{k}_1, \vec{k}_2) = -\frac{2a(\vec{k}_2)}{\pi s_1(\vec{k}_1) k_1} \quad (3.8b)$$

and

$$K_{22}(k_2, k_2') = K_{22}^{(0)}(\vec{k}_2, \vec{k}_2') + \frac{1}{r}K_{22}^{(1)}(\vec{k}_2, \vec{k}_2'), \quad (3.9)$$

$$K_{22}^{(0)}(\vec{k}_2, \vec{k}_2') = \frac{1}{\pi} \text{sgn}(\vec{k}_2) \text{sgn}(\vec{k}_2') \ln \left| \frac{1 - \vec{k}_2 \vec{k}_2' + s_2(\vec{k}_2) s_2(\vec{k}_2')}{\vec{k}_2 - \vec{k}_2'} \right|, \quad (3.9a)$$

$$K_{22}^{(1)}(\vec{k}_2, \vec{k}_2') = \frac{2a(\vec{k}_2)}{\pi a(\vec{k}_1) a(\vec{k}_2')}, \quad (3.9b)$$

where $s_2(\vec{k}_2) = (\vec{k}_2^2 - 1)^{1/2}$ and $a(\vec{k}_2) = \cosh^{-1}|\vec{k}_2|$.

A characteristic feature of the above solutions is that $K_{12}^{(1)}(\vec{k}_1, \vec{k}_2)$ are a simple product of $s_1^{-1}(\vec{k}_1)$ or $a(\vec{k}_2)$. Therefore their contributions in Eq. (2.9) and (2.12) are formally integrated and combined with their inhomogeneous term $\rho^b(k_1)$ or $\rho^b_n(k_2)$ (and $e_i(k_i)$). For example we define and evaluate

$$\tilde{\rho}_1^b(\vec{k}_1) \equiv k_F \left\{ \rho^b(k_1) + \frac{1}{r} \left[ \int d\vec{k}_1 K_{12}^{(1)}(\vec{k}_1, \vec{k}_1') \rho^b(\vec{k}_1') + \int d\vec{k}_2 K_{22}^{(1)}(\vec{k}_1, \vec{k}_2) \rho(\vec{k}_2) \right] \right\}$$

$$= \frac{d}{\pi s_1(\vec{k}_1)} \quad (3.10a)$$

To derive the final expression we have made use of Eqs. (2.2), (2.3) and (2.10a) as

$$d = \int dk_1 \rho(k_1) + \int dk_2 \rho(k_2)$$

$$= \int dk_1 dk_1' K_{11}(k_1, k_1') \left\{ \frac{1}{2\pi} \rho^b(k_1') \right\} + \int dk_2 \left\{ 1 + \int dk_1 K_{21}(k_2, k_1) \right\} \rho(k_2)$$

$$= \int d\vec{k}_1 \tilde{\rho}_1^b(\vec{k}_1)$$

with $\int d\vec{k}_1 K_{21}^{(0)}(\vec{k}_1) = 1 + \int d\vec{k}_1 K_{21}^{(0)}(\vec{k}_2, \vec{k}_2) = 0$. Similarly, but without the prefactor $k_F$ in (3.10a), we define $\tilde{\rho}_2^b(\vec{k}_2)$ and obtain

$$\tilde{\rho}_2^b(\vec{k}_2) = \frac{d}{\pi} a(\vec{k}_2). \quad (3.10b)$$
Thus Eq. (2.9) is reduced to
\begin{align}
\bar{\rho}_1(\vec{k}_1) &\equiv k_F \rho(\vec{k}_1) = \bar{\rho}_1^b(\vec{k}_1) - \int d\vec{k}_1' K_{11}^{00}(\vec{k}_1, \vec{k}_1') g_1(\vec{k}_1') \bar{\rho}_1(\vec{k}_1') \\
&\quad + \int d\vec{k}_2' K_{12}^{00}(\vec{k}_1, \vec{k}_2') g_2(\vec{k}_2') \bar{\rho}_2(\vec{k}_2'), \tag{3.11a}
\end{align}
\begin{align}
\bar{\rho}_2(\vec{k}_2) &\equiv \rho_n(\vec{k}_2) = \bar{\rho}_2^b(\vec{k}_2) - \int d\vec{k}_1' K_{21}^{00}(\vec{k}_2, \vec{k}_1') g_1(\vec{k}_1') \bar{\rho}_1(\vec{k}_1) \\
&\quad + \int d\vec{k}_2' K_{22}^{00}(\vec{k}_2, \vec{k}_2') g_2(\vec{k}_2') \bar{\rho}_2(\vec{k}_2), \tag{3.11b}
\end{align}
where $g_i(\vec{k}_i)$ are defined by
\begin{align}
g_1(\vec{k}_1) &\equiv k_F^{-1} \frac{\rho_n(\vec{k}_1)}{\rho(\vec{k}_1)} = k_F^{-1} \exp\{\bar{\beta} \bar{\varepsilon}(\vec{k}_1)\}, \tag{3.12a}
g_2(\vec{k}_2) &\equiv k_F \frac{\rho(\vec{k}_2)}{\rho_n(\vec{k}_2)} = k_F \exp\{-\bar{\beta} \bar{\varepsilon}(\vec{k}_2)\} \tag{3.12b}
\end{align}
and are shown below to be of the order of $O(h^0)$.

We regard $\bar{\rho}_i^b(\vec{k}_i)$ in Eq. (3.11), instead of $\rho^b(\vec{k}_1)$ and $\rho^b_n(\vec{k}_2)$ in Eq. (2.9), the bare density of states of the $i$-th excitation in the $k$-space, and then define its momentum $\tilde{p}_i(\vec{k}_i)$ by
\begin{align}
\tilde{p}_1(\vec{k}_1) &\equiv 2\pi \int_{k_1}^{k_{11}} d\vec{k}_1' \tilde{p}_1^b(\vec{k}_1') = 2 d\sgn(\vec{k}_1) \cos^{-1}|\vec{k}_1|, \tag{3.13a}
\tilde{p}_2(\vec{k}_2) &\equiv 2\pi \int_{k_2}^{k_{12}} d\vec{k}_2' \tilde{p}_2^b(\vec{k}_2') = 2 d\sgn(\vec{k}_2) \{a(\vec{k}_2) \cosh a(\vec{k}_2) - \sinh a(\vec{k}_2)\}. \tag{3.13b}
\end{align}
Here the upper (lower) limit $-1$ has to be used for $\vec{k}_1<0$ ($\vec{k}_2<-1$). Actually $\tilde{p}_1(\vec{k}_1)$ is the wave-number of phonon, whose Brillouin zone is appropriately chosen such that $\tilde{p}_1(k_F) - \tilde{p}_1(-k_F) = 2\pi d = 2\pi/a$.

With this specification we introduce
\begin{align}
\tilde{A}_{ii}(\tilde{p}_i, \tilde{p}_j) &\equiv \left(-\frac{d\tilde{p}_i}{dk_i}\right)^{-1} K_{ii}^{00}(\vec{k}_i, \vec{k}_i'), \quad i = 1, 2, \tag{3.14}
\tilde{A}_{ij}(\tilde{p}_i, \tilde{p}_j) &\equiv -\left(-\frac{d\tilde{p}_i}{dk_i}\right)^{-1} K_{ij}^{00}(\vec{k}_i, \vec{k}_j), \quad i \neq j. \tag{3.15}
\end{align}
Then, for example, we obtain
\begin{align}
\tilde{A}_{22}(\tilde{p}_1>0; \tilde{p}_2'<0) &\equiv \frac{1}{\pi da(\vec{k}_2)} \tanh^{-1}\left\{\frac{\tanh a(\vec{k}_2)}{2}, \tanh a(\vec{k}_1)\right\}, \tag{3.16}
\end{align}
which exactly coincides with the phase-shift function due to Theodorakopoulos and Mertens,\textsuperscript{17} or more explicitly, the spatial shift of a right-going soliton $a(\vec{k}_2>1)$ due to a collision with a left-going soliton $a(\vec{k}_2'<-1)$, obtained by means of the classical inverse scattering method.\textsuperscript{9} Similarly confirmed is the coincidence of other phase-shift functions $\tilde{A}_{ij}(\tilde{p}_i, \tilde{p}_j)$ with $K_{ij}^{00}(\vec{k}_i, \vec{k}_j)$ except for $K_{12}^{00}(\vec{k}_1, \vec{k}_1')$, phonon-phonon scattering effect,
whose corresponding phase-shift function has not yet been obtained by the classical inverse scattering method.

We have thus shown that with the proper definition of the momenta Eq. (3.11) from the YY theory exactly coincides with Eq. (2.20) of the simple-minded EIGP scheme. (The coincidence between \( g_\iota (\tilde{k}_1) \) and \( n_\iota (\rho_1) \) is also confirmed by Eqs. (3.12), (2.11) and (2.18).) We emphasize here a quite interesting fact that the value \( k_F (or \tilde{k}_F = k_F / C) \) can be still completely arbitrary in the above argument. Even Eqs. (2.2) and (2.3) cannot be a condition to specify \( k_F \). We have to look for other reasoning to specify \( k_F \), or to separate the contributions to thermodynamic quantities into phonon and soliton parts.

3.3. Energies

To investigate Eq. (2.12) of the Toda lattice let us first define \( \tilde{\varepsilon}_\iota^b (k_i) \), which is the sum of \( \tilde{\varepsilon}_\iota (k_i) \) and the contributions from the \( K_\iota^b (\tilde{k}_i, \tilde{k}_j) \) parts in Eq. (2.12):

\[
\tilde{\varepsilon}_\iota^b (k_i) = \tilde{\varepsilon}_\iota (k_i) + \frac{1}{rk_F^2} \int \! dk'_i K_\iota^b (\tilde{k}_1, \tilde{k}_i') f_\iota (k'_i) - \frac{1}{rk_F^2} \int \! dk_2 K_\iota^b (\tilde{k}_1, \tilde{k}_2) f_\iota (k_2)
\]

\[
= 2k_F \{ s_\iota (\tilde{k}_1) + \lambda / s_\iota (\tilde{k}_1) \}, \tag{3.17a}
\]

where

\[
\lambda = -\frac{1}{2} + \frac{2}{r} \left( \bar{\mu}^* + \bar{\eta}^* - \frac{1}{4} \right) , \tag{3.18}
\]

\[
\bar{\eta}^* = \frac{1}{\pi} \int \! dk_1 \frac{1}{s_\iota (\tilde{k}_1)} \bar{f}_\iota^*(\tilde{k}_1) - \frac{1}{\pi} \int \! dk_2 a(\tilde{k}_2) \bar{f}_\iota (\tilde{k}_2) , \tag{3.19}
\]

\( \bar{\mu}^* \equiv \bar{\mu} / 2k_F^2 \), \( \bar{f}_\iota^*(\tilde{k}_1) \equiv f_\iota (k_1) / 2k_F^2 \), and \( \bar{f}_\iota (\tilde{k}_2) \equiv f_\iota (k_2) / 2k_F \). It turns out that \( \bar{f}_\iota (\tilde{k}_1) \sim O(\hbar^0) \). Similarly \( \tilde{\varepsilon}_\iota^b (k_2) \) is defined and evaluated as

\[
\tilde{\varepsilon}_\iota^b (k_2) = \tilde{\varepsilon}_\iota (k_2) - \frac{1}{rk_F^2} \int \! dk_1 K_\iota^b (\tilde{k}_2, \tilde{k}_1) f_\iota (k_1) + \frac{1}{r} \int \! dk'_2 K_\iota^b (\tilde{k}_2, \tilde{k}_2') f_\iota (k_2')
\]

\[
= 2k_F \left\{ \frac{1}{4} \sinh 2a(\tilde{k}_2) - \left( \frac{1}{2} + \lambda \right) a(\tilde{k}_2) \right\} , \tag{3.17b}
\]

where \( \lambda \) is defined above. Since in the present argument all the energies are normalized by \( \hbar^2 r^2 / 2m \), and since \( k_F \sim O(\hbar^{-1}) \) is assumed, \( \varepsilon_\iota^b (k_1) \) and \( \varepsilon_\iota^b (k_2) \) in the original unit are proportional to \( \hbar \) and \( \hbar^0 \), respectively. These are the proper dependences on \( \hbar \) of the phonon and soliton energies.

It is natural then to define the following quantities to derive the formulae in the classical limit, which are free from \( \hbar \):

\[
\bar{E}_\iota (\tilde{k}_1) = \frac{\bar{E}_\iota (k_1)}{2k_F} = \frac{\bar{E}_\iota^b (k_1)}{2k_F} , \quad \bar{E}_\iota^* (\tilde{k}_1) \equiv \frac{\bar{E}_\iota^b (k_1)}{2k_F} , \tag{3.20a}
\]

\[
\bar{E}_\iota^b (\tilde{k}_2) = \frac{\bar{E}_\iota^b (k_2)}{2k_F^2} = \frac{\bar{E}_\iota^b (k_2)}{2k_F^2} , \quad \bar{E}_\iota^b (\tilde{k}_2) \equiv \frac{\bar{E}_\iota^b (k_2)}{2k_F^2} , \tag{3.20b}
\]

\[
\beta \equiv 2k_F^2 \bar{\beta} = \bar{k}_F^2 E_0 \beta^{or} . \tag{3.20c}
\]

Here the suffix \( or \) indicates the energy measured in the original unit and \( E_0 \) is defined below Eq. (3.2). With these normalizations we obtain at once that
\[ f_1(k_i) = -\frac{2k_F^2}{\beta} \ln \left[ 1 - \exp \left( -\frac{\beta E_1(k_i)}{k_F} \right) \right] \approx \frac{2k_F^2}{\beta} \ln \left( \frac{\beta E_1(k_i)}{k_F} \right), \]

or \( \tilde{f}_1(k_i) \) in Eq. (3.19) becomes

\[ \tilde{f}_1(k_i) = -\frac{1}{\beta} \left[ \ln \frac{\beta}{k_F} + \ln E_1(k_i) \right] \approx -\frac{1}{\beta} \ln \frac{\beta}{k_F} + \tilde{f}_1(k_i). \quad (3.21a) \]

When Eq. (3.21a) is substituted into Eq. (2.12) with \( K_{ij} = K_{ij}^{(0)} \), the constant \((2k_F^2/\beta) \ln(\beta/k_F)\) appears in Eq. (2.12b) but not in Eq. (2.12a). This constant can be regarded as a shift of the soliton chemical potential. In other words, if we define \( \tilde{E}_2(k_2) \) by

\[ \tilde{E}_2(k_2) = \tilde{E}_2(k_2) + \beta^{-1} \ln(\beta/k_F), \quad (3.22) \]

we obtain the equations for \( \tilde{E}_i(k_i) \) which are free from \( h \):

\[ \tilde{E}_1(k_1) = \tilde{\epsilon}_1^*(k_1) + \int d\tilde{k}_1' K_{11}^{(0)}(k_1, \tilde{k}_1') \tilde{f}_1(k_1') - \int d\tilde{k}_2 K_{12}^{(0)}(k_1, \tilde{k}_2) \tilde{f}_2(k_2), \quad (3.23a) \]

\[ \tilde{E}_2(k_2) = \tilde{\epsilon}_2^*(k_2) - \int d\tilde{k}_1 K_{21}^{(0)}(k_2, \tilde{k}_1) \tilde{f}_1(k_1) + \int d\tilde{k}_2' K_{22}^{(0)}(k_2, \tilde{k}_2') \tilde{f}_2(k_2'), \quad (2.23b) \]

where \( \tilde{f}_1(k_1) \) is given by Eq. (3.21a) and \( \tilde{f}_2(k_2) \) by

\[ \tilde{f}_2(k_2) = \frac{f_2(k_2)}{2k_F} = -\frac{k_F}{\beta} \ln \left[ 1 + \beta \exp \left( -\beta \tilde{E}_2(k_2) \right) \right] \approx -e^{-\beta \tilde{E}_2(k_2)}. \quad (3.21b) \]

The effective bare energies \( \tilde{\epsilon}_i^*(k_i) \) without the phase-shift effects due to \( K_{ij}^{(0)}(k_i, k_j) \) are given by the curly brackets in Eq. (3.17).

The parameter \( \lambda \) in Eq. (3.17) is related to the pressure of the system through Eqs. (2.6) and (2.15). In terms of the variables introduced above Eq. (2.15) becomes

\[ \bar{A} = \frac{2k_F^2}{\rho} \left( \frac{\tilde{\rho}}{4} + \tilde{\eta}^* \right). \quad (3.24) \]

Therefore from Eq. (2.6) (2C^2 is subtracted from its l.h.s.) we obtain

\[ \lambda = 2(\rho + 1) k_F^{-2} - 1/2, \quad (3.25) \]

where \( \rho = \tilde{\rho}/2C^2 \) (\( \tilde{\rho} \) in Mertens' scale).

We have thus obtained a closer correspondence between Eq. (3.23) in the TCBA scheme and Eq. (2.19) in the EIGP scheme, from which \( h \) associated with the phonon energy is eliminated in a similar way as described above. The arguments up to this point still do not rely on any explicit value of \( k_F \). The correspondence between Eqs. (3.23) and (2.19) becomes complete if \( \tilde{\epsilon}_i^*(k_i) \) in the former agrees with \( e_i(p_i) \) in the latter. In the simple-minded phenomenology the bare energy \( e_i(p_i) \) has not to be singular. These two requirements lead to the condition \( \lambda = 0 \), since otherwise \( \tilde{\epsilon}_i^*(k_i) \) becomes singular at \( k_i \rightarrow 1 \) (Eq. (3.17a)). The condition specifies the value \( k_F \) through Eq. (3.25):

\[ k_F^{-2} = 4(1 + \rho). \quad (3.26) \]

The phonon bare energy then becomes

\[ \tilde{\epsilon}_1^*(k_1) \rightarrow \tilde{\epsilon}_1^*(k_1) = s_1(k_1) = \sin \left( \pi \tilde{\rho}_1(k_1)/2 \right), \quad (3.27a) \]
where Eq. (3.13a) has been used to derive the last equality with $a = 1/d$. Similarly the soliton bare energy becomes

$$\tilde{e}_{2}^{b}(k_{s}) \rightarrow \tilde{e}_{2}^{b}(\tilde{k}_{s}) = \frac{1}{4} \sinh 2a(\tilde{k}_{s}) - \frac{1}{2} a(\tilde{k}_{s}).$$ (3.27b)

These expressions in terms of $\tilde{k}_{s}$ are identical to those obtained at zero temperature.\(^{12}\)

In order to consider the physical meaning of the exact correspondence between the two schemes thus obtained, let us rewrite the soliton bare energy given by Eq. (3.27b) in the original unit $e_{2}^{b,\text{or}}(\tilde{k}_{s})$:

$$\frac{e_{2}^{b,\text{or}}(\tilde{k}_{s})}{E_{s}} = \tilde{k}_{s}^{2} \tilde{e}_{2}^{b}(\tilde{k}_{s}) = (1 + p) \{ \sinh 2a(\tilde{k}_{s}) - 2a(\tilde{k}_{s}) \}. \quad (3.28)$$

Similarly its momentum of Eq. (3.13b) is given by

$$\frac{p_{s}^{\text{or}}(\tilde{k}_{s})}{p_{s}} = \tilde{k}_{s}^{2} \tilde{p}_{2}(\tilde{k}_{s}) = 2d(1 + p)^{1/2} \{ a(\tilde{k}_{s}) \cosh a(\tilde{k}_{s}) - \sinh a(\tilde{k}_{s}) \}, \quad (3.29)$$

where $p_{s} = ma_{0}/\gamma$. These bare energy and momentum are those of solitons on a lattice with the lattice distance $1/d$ under the pressure $p$. The Toda potential which realizes such solitons and the lattice distance is written as

$$\tilde{V}(r) = \frac{m a_{0}^{2}}{\gamma} \left[ e^{-(r - r_{0})} + (1 + p) r \right] \quad (3.30a)$$

with $d\tilde{V}/dr = 0$ at $r = 1/d$, or

$$\tilde{r}_{0} = \ln(1 + p) + 1/d, \quad (3.30b)$$

where the length is still scaled by $\gamma$. These observations lead us to the following interpretation. In the derivation of the TCBA scheme we start with the original potential (3.1) under a given lattice distance $1/d$, and end up with the effective bare energy $\tilde{e}_{2}^{b}(\tilde{k}_{s})$ after the proper renormalization of the phase-shift interaction effects, thereby the thermal expansion effect or/and the pressure effect is automatically taken into account. In the simple-minded EIGP scheme, on the other hand, we implicitly assume the effective Toda potential of Eq. (3.30) with an appropriate $\tilde{r}_{0}$, which is a function of $(1/d, T)$ or $(p, T)$ according to the thermodynamic constraint imposed.

3.4. Relation with Opper’s solution

In order to solve Eq. (2.4) of the Toda lattice in the classical limit, Theodorakopoulos\(^{16}\) has introduced the transformation

$$\varepsilon(k) \equiv \varepsilon(k)/2C^{2} = \varepsilon^{*}(k) + \frac{1}{\beta} \ln \frac{k_{F}}{\beta}$$ (3.31)

for all the value of $k$, and let $x_{F}$ go to infinity in the classical limit. Here energies without the bar indicate those in the original unit scaled by $E_{s}$; namely,

$$\beta^{-1} = T = \frac{T^{\text{or}}}{E_{s}} = \frac{T}{2C^{2}} = \frac{T}{k_{F}^{2} T_{c}} \equiv \tilde{T}. \quad (3.32)$$

By the transformation Eqs. (2.4) and (2.6) are reduced to
\[
e^*(\vec{k}) = \frac{1}{2} \vec{k}^2 - \mu_x + \frac{C}{\chi_F} \int d\vec{k}' T(\vec{k} - \vec{k}') e^{-\beta e^*(\vec{k}')}, \tag{3.33}
\]

\[
1 + \rho = \frac{C}{2\pi\chi_F} \int d\vec{k} e^{-\beta e^*(\vec{k})}, \tag{3.34}
\]

where \(\vec{k} \equiv k/C\) and \(\mu_x = \mu - \beta^{-1}\ln(\chi_F/\beta)\). He solved these equations numerically and claimed that \(e^*(k) = 0\) specifies \(k_F\) and the phonon (soliton) energy is given by \(-e^*(k)\) with \(|k| < k_F\). \(e^*(k)\) with \(|k| > k_F\).

Later Opper\(^{18}\) succeeded in solving Eqs. (3.33) and (3.34) analytically. In the present notations the solution is written as

\[
e^{-\beta e^*(k)} = \frac{2\pi}{C} \beta^{1/2} \phi_\rho(x = \beta^{1/2} \vec{k}), \tag{3.35}
\]

where

\[
\phi_\rho(x) = \frac{e}{\pi} \text{Re} \left[ \frac{D_{-\rho^{-1}}(-ix)}{D_{-\rho}(-ix)} \right], \tag{3.36}
\]

\[
\rho = (1 + \rho) \overline{\beta} \tag{3.37}
\]

and \(D_{\nu}(z)\) is the parabolic cylinder function.\(^{18}\) A brief explanation of this solution is given in the Appendix. From the solution he reproduces the chemical potential \(\mu^*(\rho, T)\) in a closed form which agrees exactly with Toda’s result:\(^2\)

\[
\mu^*(\rho, T) = (\bar{\mu} - 2C^2 r_0)/2C^2 = r_0 \rho - \beta^{-1}\ln C + \frac{\rho}{\beta} \ln \beta + \frac{1}{2\beta} \ln(2\pi \beta) - \frac{1}{\beta} \ln \Gamma(\rho) \tag{3.38}
\]

\[
\cong r_0 \rho + (1 + \rho)(1 + \rho) \ln(1 + \rho) + \frac{1}{\beta} \ln\left(\frac{h\omega}{E}\right) + \frac{1}{2\beta} \ln \beta \rho
\]

\[
- \frac{1}{12\beta \rho} + \frac{1}{360\beta \rho^3} - \cdots, \tag{3.38'}
\]

where \(\Gamma(\rho)\) is the gamma function and Eq. (3.38') is the asymptotic expansion at low temperatures (\(\beta, \rho \gg 1\)).

An interesting feature of Opper’s solution is that the parameter \(x_F\) does not appear at all in the final results. Therefore we can easily relate \(\bar{E}_i(\vec{k}_i)\) in the present work with Opper’s solution through Eq. (2.11), as explicitly shown in the Appendix (Eq. (A.7)). This means that the two methods of the classical thermodynamics by Theodorakopoulos\(^{19}\) and in the present work are essentially identical. When the value \(k_F\) given by Eq. (3.26) is adopted, \(\bar{E}_i(\vec{k}_i)\) are given by

\[
\bar{E}_1(\vec{k}_i) = \pi \rho^{-1/2} \phi_\rho(x = 2\rho^{1/2} |\vec{k}_i|), \tag{3.39a}
\]

\[
\bar{E}_2(\vec{k}_2) = -\frac{1}{4\rho} \ln \{\pi \rho^{-1/2} \phi_\rho(x = 2\rho^{1/2} |\vec{k}_2|)\}. \tag{3.39b}
\]

Substituting these solutions into Eq. (3.23) with (3.21), we confirm numerically \(\bar{e}_i^*(\vec{k}_i) = \bar{e}_i^{\rho}(\vec{k}_i)\), which means that the condition \(\lambda = 0\), or Eq. (3.26) does not conflict with Opper’s solution.

We plot in Fig. 1 \(\bar{E}_i(\vec{k}_i)\) with \(\rho = \infty\) and \(\rho = 10\). The former is the phonon and soliton excitations at \(T = 0\), and is equal to \(\bar{e}_i^{\rho}(\vec{k}_i)\). Notice that \(\phi_\rho(x)\) is analytic for a finite \(\rho\).
In Fig. 2 the effective phonon energy $\tilde{E}_1(\tilde{k})$ is plotted as a function of the normalized wave number $\tilde{p}_1(\tilde{k})/2d$. For long wave phonons ($\tilde{k}_0 \approx 1$) the phase-shift interaction effects by other phonons and solitons, $\Delta E_{ph-ph}$ and $\Delta E_{ph-sol}$, are both large. They cancel with each other, but not exactly, and yield a finite shift of $\tilde{E}_1(\tilde{k})$ from the bare energy $\tilde{e}_1^{b}(\tilde{k})$. This last result will be discussed in § 4.

Before closing this subsection we discuss the specification of the key parameter $k_F$ or $\tilde{k}_F$. At zero temperature the existence of such a critical value as well as its explicit value are derived by Oppen's solution since $d\Phi_\rho/dx$ is discontinuous at $x = 2\rho^{1/2}$ in the limit $\rho \to \infty$ (see Fig. 1 and Eq. (A-10) in the Appendix). The $k$-space is separated at $|k| = k_F^{(0)} = \tilde{k}_F^{(0)}C$, where $k_F^{(0)}$ is given by Eq. (3.26). We emphasize that this $k_F^{(0)}$ obtained after we have moved to the classical thermodynamics is identical to that which specifies the ground state of the original quantum system.\(^{12,13}\) At finite temperatures $\Phi_\rho(x)$ becomes an analytic function of $x$, so that Oppen's solution alone does not specify $\tilde{k}_F$. The requirement that the two schemes, TCBA and EIGP, have to coincide with each other specifies $\tilde{k}_F$ in the classical thermodynamics.

It is clear from Eq. (3.26) that $k_F$ thus determined is independent of $T$ when $\rho$ is fixed, while it is $T$-dependent when the system length (or $d$) is fixed. The present $k_F$ does not agree with that defined by Theodorakopoulos\(^{19}\) nor with the classical limit of $k_F$ of Hader and Mertens.\(^{14}\) In particular if we adopt the latter specification

$$d = \int_{-k_F}^{k_F} dk\{\rho(k) + \rho_n(k)\} \tag{3.40}$$

$\tilde{k}_F = k_F/C$ vanishes in the classical limit, since $\rho_n(k)$ is of the order $O(h^0)$ (see Eq. (3.12) and relating discussion).
3.5. Classical thermodynamics

Given the well-defined \( k_F \) our next task is to divide the contributions to thermodynamic quantities into soliton and phonon parts. Let us first consider the chemical potential \( \mu^* \), or the Gibbs free energy per particle, as a function of \( p \) and \( T \). It is obtained from Eqs. (2.6) and (3.24) as

\[
\mu^*(p, T) = \mu_0 + \mu_{hp} + \mu_{sp} + \mu_s,
\]

where

\[
\mu_0(p) = r_0 p + 1 + p - (1 + p) \ln(1 + p),
\]

\[
\mu_{hp}(p, T) = \frac{1}{\beta} \ln \left( \frac{\hbar \omega}{E_s} \right) + \frac{1}{\beta} \ln \beta,
\]

\[
\mu_{sp}(p, T) = \frac{1}{2\beta} \ln(1 + p) - \frac{1}{\pi \beta} \int d\vec{k}_1 s_{1s}(\vec{k}_1) \ln \{ 2E_s(\vec{k}_1) \},
\]

\[
\mu_s(p, T) = \frac{4p}{\pi \beta} \int d\vec{k}_2 \alpha(\vec{k}_2) \exp \{ - \beta E_s(\vec{k}_2) \}.
\]

Above \( \mu_0 \) is the chemical potential at \( T = 0 \), and \( \mu_s \) comes out from the last term of Eq. (2.15) and is regarded as the soliton contribution. The remaining terms are subdivided into the harmonic phonon part \( \mu_{hp} \) and that due to the anharmonicity of the phonons \( \mu_{sp} \).

Comparing Eq. (3.41) with Eq. (3.38) one notices that

\[
\left\{ \mu_{hp} - \frac{1}{2\beta} \ln(1 + p) \right\} + \mu_s = \frac{1}{\beta} \left( \frac{1}{12p} - \frac{1}{360p^3} + \cdots \right).
\]

With the above specification we can evaluate the soliton contribution in various thermodynamic quantities. For example the soliton specific heat \( C_{p,s}(T) \) \( \equiv - T (\partial^2 \mu_s / \partial T^2)_p \) is numerically evaluated and shown in Fig. 3. Its asymptotic expansion at low temperatures is hardly obtained due to the reason mentioned below Eq. (A.9) in the Appendix. At a first glance it is of interest that \( C_{p,s}(T) \) exhibits a round peak at low temperatures. However the peak is compensated by the anharmonicity of the phonon, and the total \( C_p(T) \) exhibits a simple power dependence on \( T \) as Toda's result \(^2\) predicts. The circumstances are the same for any other thermodynamic quantities. It seems hard to distinguish the soliton contribution in the thermodynamic quantities.

\[\text{Fig. 3. Specific heat of the Toda lattice under fixed pressure } C_p(T), \text{ and the soliton contribution (plus one) to it } C_{p,s}(T). \text{ Note the harmonic phonon contribution is unity (independent of } T).\]

§ 4. Discussion

We have argued classical thermodynamics of the Toda lattice starting from the corresponding quantum statistical mechanics formulated by the Bethe
ansatz method. By the appropriate rearrangement of the Yang-Yang equation the two-
component Bethe ansatz (TCBA) scheme is constructed following the method developed
in our previous work I. The classical limit of this TCBA scheme is analyzed, and solved
with the aid of Oppé’s solution.\cite{10} If the key parameter $k_F$ is properly chosen, the
resultant coupled equations which determine the effective soliton and phonon energies are
identical to those expected from the simple-minded EIGP scheme, in which effects of the
phase-shift interactions are evaluated by means of the classical inverse scattering method.
In this sense, we believe, the present construction of the two-component gas system (or the
specification of the soliton and phonon modes) is a most natural, and reasonable as for the
classical thermodynamics. A certain singular contribution of solitons to thermodynamic
quantities is obtained, but it is mostly compensated by the contribution of the anharmonic
ity of phonons so that it seems hard to distinguish the soliton contribution thermodynamically.

These features, i.e., the way of specification of modes and the difficulty of their
distinction in thermodynamic quantities, are thought rather common in classical
thermodynamics of nonlinear integrable systems whose counterpart in quantum statistical
mechanics can be formulated by the YY equations of the form such as Eq. (2.4). Another
example is the system described by the nonlinear Schrödinger equation, whose counter-
part is a Bose gas with repulsive $\delta$-function-type interactions as discussed in I. Similar
features are also expected if we try to describe classical thermodynamics of the soliton-
free sector of the sine-Gordon system in terms of phonons and breathers,\cite{19} though the
corresponding YY equation is more complicated than Eq. (2.4).\cite{9,10} Actually its classical
thermodynamics can be interpreted as that of interacting phonons, but at the same time
a part of their contributions can be reinterpreted as those of breathers, or the phonon
bound states.\cite{20}

Lastly it is pointed out that at finite temperatures the effective energy $\tilde{E}_t(\hat{k}_1)$ obtained
in this work does not vanish even at $\hat{k}_1 = 1$ for which the momentum (or the wave number)
$\hat{p}_1$ equals zero. This is seen in Fig. 2 and also from Eq. (3.39) combined with the fact that
Oppé’s function $\phi_\rho(x)$ is positive finite for finite $\rho$. It is reasonable since $\tilde{E}_t(\hat{k}_1)$ is
directly related to the number density of the mode (see Eq. (2.18)), rather than to the
dynamical frequency of the mode. The problem of dynamics is beyond the scope of the
present work. At the moment therefore we cannot make a comment on the relation
between $\tilde{E}_t(\hat{k}_1)$ (or $\tilde{E}_t^I(\hat{k}_1)$) and the dispersion relation obtained by the molecular
dynamics simulation at finite temperatures.\cite{21} We expect, however, that the thermal
population of the mode is properly given by the present $\tilde{E}_t(\hat{k}_1)$.

Appendix

We briefly discuss Oppé’s solution.\cite{10} In terms of the variables

\[ x \equiv \beta^{1/2} \hat{k}, \]

\[ \phi(x) = \xi e^{-\beta e^{*(\hat{k})}}, \quad \xi = C\beta^{1/2}/2\pi k_F, \quad (A.1) \]

Eqs. (3.33) and (3.34) are written as
\[ \ln \phi(x) - \beta \bar{\mu}_e = -\frac{1}{2} x^2 + 2 \int_{-\infty}^{\infty} dx' \ln |x - x'| \phi(x'), \tag{A.2} \]
\[ \rho = \int_{-\infty}^{\infty} dx \phi(x), \tag{A.3} \]

where \( \bar{\mu}_e = \mu_e + \beta^{-1} \ln \xi - (1 + p)(\rho_0 + \ln \beta) \). Oppen finds the solution for Eqs. (A.2) and (A.3) as
\[ \phi_\rho(x) = \frac{1}{\pi} \frac{\text{Im} d}{dx} [\ln f_\rho(x)], \tag{A.4} \]
\[ f_\rho(x) = \int_0^{\infty} dt e^{ix(t - (t^2/2))} t^{-1} = \Gamma'(\rho) e^{-x^2/4} D_{-\rho}(-ix), \tag{A.5} \]

where \( D_{-\rho}(-ix) \) is the parabolic cylinder function.\(^{18}\) By the recurrence formula for \( D_{-\rho}(-ix) \) Eq. (A.4) reduces to Eq. (3.36) in the text. Note that \( \exp\{-\beta \varepsilon(k)\} \) is free from \( \chi_F \)
\[ e^{-\beta \varepsilon(k)} = \frac{\beta}{\chi_F} e^{-\beta \varepsilon(k)} = \frac{2\pi \beta^{1/2}}{C} \phi_\rho(x). \tag{A.6} \]

For phonons this equals the inverse of the r.h.s. of Eq. (2.11),
\[ \frac{2\pi \beta^{1/2}}{C} \phi_\rho(x) = \exp(\frac{\beta \varepsilon_1(k)}{\hbar K_F}) - 1 \approx \frac{\hbar K_F \varepsilon_1(k)}{C}. \tag{A.7} \]

With \( \hbar k_F \) given by Eq. (3.26), Eq. (A.7) reduces to Eq. (3.39a). Equation (3.39b) is similarly derived.

The function \( D_{-\rho}(-ix) \) in Eq. (3.36) is evaluated by its integral representation of Eq. (A.5):
\[ D_{-\rho}(-ix) = \Gamma'(-1) e^{x^2/4} \int_0^{\infty} dt \exp\{g_\rho(t, x)\}, \tag{A.8} \]
\[ g_\rho(t, x) = -\frac{t^2}{2} + ixt + \rho \ln t. \tag{A.9} \]

In case \( x^2 > 4 \rho \), \( g_\rho(t, x) \) has a local maximum (minimum) at \( t = i \tau_\rho^- (i \tau_\rho^+) \) along the imaginary axis where \( \tau_\rho^0 = \frac{x \pm (x^2 - 4 \rho^2)^{1/2}}{2} \). Therefore the integral in Eq. (A.8) is evaluated along the path shown in Fig. A1. At low temperatures \( (\rho \gg 1) \), the integrand can be approximated by simple Gaussians around \( t = i \tau_\rho^0 \). This is not the case for \( x \approx 2 \rho^{1/2} \), i.e., \( |k_F| \approx k_F \), which is the reason why we can hardly obtain the asymptotic expansion for thermodynamic quantities. Only at the zero temperature limit we can neglect contribution from such fine structures and obtain
\[ \pi \rho^{-1/2} \phi_\rho(x) \approx \begin{cases} (1 - y^2)^{1/2}, & y < 1 \\ \frac{1}{2} \exp[-2 \rho (y(y^2 - 1) - \cosh^{-1}y)], & y > 1, \end{cases} \tag{A.10} \]

where \( y = x/2 \rho^{1/2} \).

Fig. A1. Integral path of Eq. (A.8) in case \( x^2 > 4 \rho \).
References