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Thermodynamics of the quantum Toda lattice

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Abstract. Thermodynamics of the quantum Toda lattice is studied based on Gutzwiller's quantization condition and Yang–Yang's thermodynamic formulation. It is shown that Gutzwiller's quantization condition becomes identical to the Bethe ansatz equation in the thermodynamic limit. We have calculated the thermodynamic averages of the energy, higher-order conserved quantities and the specific heat. The average energy and the specific heat become close to those of the classical Toda lattice in the high temperature limit, while they are similar to those of a harmonic chain in the low temperature limit.

1. Introduction

The Toda lattice [1] is one of the most popular models of completely integrable systems [2]. Among those integrable models, many-body problems and thermodynamics are well studied for the δ -function interaction gas (nonlinear Schrödinger model) [3] and Calogero–Sutherland model [4]. On the contrary, the study of thermodynamics of the Toda lattice has been very limited. A pioneering work was done by Sutherland [5], where the Bethe ansatz was applied to the Toda lattice in the classical approximation. This approach was further pursued by Mertens [6] and Hader and Mertens [7]. They studied the thermodynamics of an open Toda lattice by employing the Bethe ansatz and the Yang–Yang method [8]. Since the open Toda lattice only has scattering states, the system was confined in a box. They treated the case that the wavefunction is very small in the region $x > 0$ where the Toda potential $V(x) = e^x \rightarrow \infty$ as $x \rightarrow \infty$. Therefore applying the Bethe ansatz is only understandable in the low momentum and low density regions.

Another way to confine the system is to couple the first and the last particles in the same way as others, i.e. to make a periodic lattice. In the thermodynamic limit $N \rightarrow \infty$, bulk properties do not depend on the method of confinement. A satisfactory formulation of the quantum periodic Toda lattice was first worked out by Gutzwiller [9]. He has developed a systematic way of quantization of the periodic Toda lattice. His quantization condition is well defined and very similar to the Bethe ansatz equation. Fowler and Frahm [10] have studied the periodic Toda lattice based on Gutzwiller's quantization condition and shown that the energy spectra are different from those given by the Bethe ansatz equation for a finite particle system. They have also suggested that Bethe ansatz would give the correct spectra in the large N limit. Meanwhile, Sklyanin [11] has combined the quantum spectral transform method (QSTM) (R -matrix formalism) and Gutzwiller's formulation and derived an equation for the spectrum of the quantum Toda lattice.

In [12], we have studied the ground state of the periodic Toda lattice and shown that Gutzwiller's quantization condition is largely simplified in the large N limit. The purpose of this paper is to extend our study of the quantum periodic Toda lattice [12] for excited

states and to formulate the thermodynamics of the Toda lattice according to the Yang–Yang formulation. We will show that Gutzwiller’s quantization condition becomes identical to the Bethe ansatz equation in the thermodynamic limit.

In section 2, we will review the formulation of the quantum Toda lattice and, in section 3, we will describe the thermodynamics of the quantum Toda lattice. Numerical methods will be explained in section 4 and those results will be discussed in section 5. Section 6 is devoted to a summary.

2. Formulation

2.1. Hamiltonian and conserved quantities

In order to make our paper self-contained, we will briefly review the Hamiltonian and the conserved quantities of the periodic Toda lattice. The Hamiltonian of the periodic N -particle Toda lattice is given in a dimensionless form as

$$H = \frac{1}{2} \sum_{i=1}^N p_i^2 + \sum_{i=1}^N \exp(x_i - x_{i+1}) \quad (2.1)$$

where we set $x_{N+1} = x_1$. Flaschka [13] has shown that the classical equations of motion can be written in a Lax form

$$\frac{dL}{dt} = [B, L] \quad (2.2)$$

where L and B are the $N \times N$ matrices,

$$L = \begin{pmatrix} b_1 & a_1 & & & a_N \\ a_1 & b_2 & a_2 & & \\ & \cdots & \cdots & \mathbf{0} & \\ & & \cdots & \cdots & \\ \mathbf{0} & a_{N-2} & b_{N-1} & a_{N-1} & \\ a_N & & a_{N-1} & b_N & \end{pmatrix} \quad (2.3)$$

$$B = \begin{pmatrix} 0 & -a_1 & & & a_N \\ a_1 & 0 & -a_2 & & \\ & \cdots & \cdots & \mathbf{0} & \\ & & \cdots & \cdots & \\ \mathbf{0} & a_{N-2} & 0 & -a_{N-1} & \\ -a_N & & a_{N-1} & 0 & \end{pmatrix} \quad (2.4)$$

and the quantities a_i and b_i are defined by

$$a_i = \frac{1}{2} \exp\left(\frac{1}{2}(x_i - x_{i+1})\right) \quad b_i = \frac{1}{2} p_i. \quad (2.5)$$

Therefore the eigenvalues of the matrix L are constants of motion and thus the coefficients of the characteristic polynomial are also constants of motion. Let us define the coefficients A_i as follows (I is $N \times N$ identity matrix):

$$\det(2\lambda I - 2L) = \sum_i A_i (2\lambda)^{N-i} - 2 \quad (2.6)$$

where $A_0 = 1$. The conserved quantities A_i are in involution with the Hamiltonian, $[H, A_i] = 0$, and also mutually in involution, $[A_i, A_j] = 0$. The quantity A_n is an n th order polynomial of the momenta and its explicit form is given by Hénon [14]:

$$A_n = (-1)^n \sum p_{i_1} p_{i_2} \cdots p_{i_k} (-X_{j_1}) (-X_{j_2}) \cdots (-X_{j_l}) \quad (n = k + 2l) \quad (2.7)$$

with $X_j = \exp(x_j - x_{j+1})$. The sum is taken over all terms with different indices $(i_1, i_2, \dots, i_k, j_1, j_1 + 1, \dots, j_l, j_l + 1)$. In the centre-of-mass (CM) system, $A_1 = -P = 0$, $A_2 = \frac{1}{2}P^2 - H = -H$. Thus the conserved quantities A_1 and A_2 have physical meanings of the total momentum and the energy, respectively. However, the quantities A_n ($n \geq 3$) do not have physical interpretation.

In quantum mechanics, the Hamiltonian \hat{H} and the conserved quantities \hat{A}_i are operators and are given by the canonical quantization, i.e. the momentum p_i is replaced by the operator $\hat{p}_i = -i\hbar(\partial/\partial x_i)$. The constant \hbar is basically arbitrary and sets the scale of the system. The advantage of the Hénon-type conserved quantities is that the ordering problems of operators $\{\hat{x}_i, \hat{p}_i\}$ do not occur.

2.2. Gutzwiller's quantization condition

In [9], Gutzwiller developed a systematic way of constructing simultaneous eigenfunctions of the operators \hat{H} and \hat{A}_i for $N = 2, 3$ and 4 particle lattices. Later, his method was extended generally for the N -particle periodic Toda lattice by employing the transfer matrix method by Pasquier and Gaudin [15]. Let us briefly summarize his algorithm of quantization. Suppose we have $N - 1$ real numbers $(E, A_3, A_4, \dots, A_N)$ and try to examine whether they are simultaneous eigenvalues of the operators \hat{H} and \hat{A}_i .

Firstly we should solve a Hill-type equation $\Delta(\kappa) = \det C = 0$, where C is a tridiagonal infinite matrix

$$C = \begin{pmatrix} \ddots & & & & & & \\ & \ddots & & & & & \\ & & 1 & \frac{(-1)^N}{D(\kappa-1)} & & & \\ & & \frac{1}{D(\kappa)} & 1 & \frac{(-1)^N}{D(\kappa)} & 0 & \\ & & & \frac{1}{D(\kappa+1)} & 1 & \frac{(-1)^N}{D(\kappa+1)} & \\ & 0 & & & \frac{1}{D(\kappa+2)} & 1 & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix} \tag{2.8}$$

with

$$D(\kappa) = (\hbar\kappa)^N + E(\hbar\kappa)^{N-2} - iA_3(\hbar\kappa)^{N-3} + A_4(\hbar\kappa)^{N-4} + iA_5(\hbar\kappa)^{N-5} + \dots + i^N A_N \tag{2.9}$$

and κ is a complex number. The equation $\Delta(\kappa) = \det C = 0$ has generally N different purely imaginary solutions κ_i ($\sum_i \kappa_i = 0$) in $-\frac{1}{2} \leq \Re(\kappa) \leq \frac{1}{2}$. In the case of $N = 2$, the Schrödinger equation of the periodic Toda lattice is the modified Mathieu equation and $\Delta(\kappa)$ is a well known Hill's determinant. In practical calculation, it is useful to rewrite Hill's determinant as

$$\Delta(i\lambda) = r_{i\lambda} r_{i\lambda-1}^* - (-1)^N r_{i\lambda}^* r_{i\lambda+1} / \{D(i\lambda)D(i\lambda + 1)\} \tag{2.10}$$

where r_κ is defined by the recursion relation

$$r_{\kappa-1} = r_\kappa - (-1)^N r_{\kappa+1} / \{D(\kappa)D(\kappa + 1)\} \tag{2.11}$$

with the boundary condition $r_\kappa \rightarrow 1$ at $\Re(\kappa) \rightarrow \infty$. The solution r_κ can be given explicitly

as a determinant of the lower-right semi-infinite part of the matrix C , i.e. $r_\kappa = \det C'$ where

$$C' = \begin{pmatrix} 1 & \frac{(-1)^N}{D(\kappa+1)} & 0 & & \\ \frac{1}{D(\kappa+2)} & 1 & \frac{(-1)^N}{D(\kappa+2)} & & \\ 0 & \frac{1}{D(\kappa+3)} & 1 & \ddots & \\ & & \ddots & \ddots & \ddots \end{pmatrix}. \quad (2.12)$$

Let $\kappa = i\lambda_j$ ($\lambda_1 < \lambda_2 < \dots < \lambda_N$) be one of the zeros of Hill's determinant, that is, Floquet's characteristic exponents. Then, Gutzwiller's quantization condition is expressed as

$$\phi_j = \arg(\hbar^{iN\lambda_j}) + \sum_k \arg(\Gamma(1 + i(\lambda_j - \varepsilon_k))) - \arg(r_{i\lambda_j}) = \frac{m\pi}{N} \pmod{\pi} \quad (2.13)$$

where $\{i\varepsilon_k\}$ ($\varepsilon_1 < \varepsilon_2 < \dots < \varepsilon_N$) are N different zeros of the polynomial $D(\kappa)$ (thus the poles of $\Delta(\kappa)$). ϕ_j is a monotonically increasing function of λ_j , i.e. $\phi_{j+1} - \phi_j = \pi(n_j + 1)$ with non-negative integers n_j [10]. These $N - 1$ non-negative integers (n_1, n_2, \dots, n_{N-1}) are quantum numbers. The integer m which is the same for all j characterizes the symmetric property of the eigenfunction and has a one-to-one correspondence to the irreducible representations of the dihedral group D_N [16]. It takes the values $m = 0, \pm 1, \pm 2, \dots, \pm(N - 1)/2$ for $N = \text{odd}$ and $m = 0, \pm 1, \pm 2, \dots, \pm(N - 2)/2, N/2$ for $N = \text{even}$. The relation of the integer m and the quantum numbers $\{n_i\}$ is discussed in [16, 17].

2.3. Open Toda lattice in a box

In this section, we will describe the quantization condition of the open Toda lattice with periodic boundary condition. The Hamiltonian of the N -particle open lattice is

$$H = \frac{1}{2} \sum_{i=1}^N p_i^2 + \sum_{i=1}^{N-1} \exp(x_i - x_{i+1}). \quad (2.14)$$

Since the open lattice has only scattering states, one must confine the system in a box with periodic boundary condition. Imposing the periodic boundary condition is equivalent to adding an interaction term $\exp(x_N - x_1 - L)$, where L is the length of the box. This is because the N th particle can interact with the $(N + 1)$ th particle beyond the box with the potential $\exp(x_N - x_{N+1})$ where one should identify $x_{N+1} = x_1 + L$. Therefore the Hamiltonian of the open lattice with periodic boundary condition is

$$H = \frac{1}{2} \sum_{i=1}^N p_i^2 + \exp(x_1 - x_2) + \dots + \exp(x_{N-1} - x_N) + \exp(x_N - x_1 - L). \quad (2.15)$$

In order to make the potential terms symmetric, let us introduce new variables $\{y_i\}$ such that

$$y_i = x_i + (N - 2i + 1) \frac{L}{2N}. \quad (2.16)$$

Then the Hamiltonian becomes

$$H = \frac{1}{2} \sum_{i=1}^N p_i^2 + e^{-L/N} \sum_{i=1}^N \exp(y_i - y_{i+1}) \quad (2.17)$$

where $y_{N+1} = y_1$. Note that the transformation (2.16) does not change the centre of mass motion, i.e. $\sum_i x_i = \sum_i y_i$. Therefore the open lattice with periodic boundary condition is

equivalent to the periodic lattice with a modified potential strength $e^{-L/N}$. In other words, the periodic lattice is a special case of the open lattice with a box length $L = 0$.

In quantum mechanics, the modified factor $e^{-L/N}$ can be absorbed by rescaling $\hbar \rightarrow \hbar e^{L/2N}$. Then one can repeat Gutzwiller's quantization procedure. In the end, one should replace the $D(\kappa)$ function of (2.9) by $D(\kappa) \rightarrow D(e^{L/2N}\kappa)$, and quantization condition (2.13) by

$$\begin{aligned} \phi_j &= \frac{1}{2}L\lambda_j + \arg(\hbar^{iN\lambda_j}) + \sum_k \arg(\Gamma(1 + i(\lambda_j - \varepsilon_k))) - \arg(r_{i\lambda_j}) \\ &= \frac{m\pi}{N} \pmod{\pi}. \end{aligned} \tag{2.18}$$

3. Thermodynamics of the Toda lattice

3.1. Ground state

In this section, we will derive the quantization condition in the thermodynamic limit, i.e. large N limit for the periodic lattice, or large N, L limit while keeping the density $D = N/L$ finite for the open lattice in a box.

In [12], we have shown the following two important properties of Hill's determinant of the periodic lattice in the large N limit.

(i) The determinant $r_{i\lambda_j}$ of the semi-infinite matrix C' (2.12) approaches to 1 and the difference decreases as $O(e^{-\alpha N})$ ($\alpha > 0$).

(ii) The j th pole $i\varepsilon_j$ and zero $i\lambda_j$ are very close and the difference decreases as $O(e^{-\beta N})$ ($\beta > 0$).

We have also carried out numerical calculations with $\hbar = 1$ and particle number $2 \leq N \leq 20$, and obtained $\alpha = 1.6 \sim 2.3$, $\beta = 1.2 \sim 1.8$. These two properties largely simplify Gutzwiller's quantization condition (2.13) in the large N limit and it becomes for the scale $\hbar = 1$

$$\phi_i = \sum_j \arg(\Gamma(1 + i(k_i - k_j))) = \frac{m\pi}{N} \pmod{\pi} \tag{3.1}$$

where we rewrite $\lambda_i = \varepsilon_i = k_i$. k_i s are so-called pseudo-momenta. We will set $\sum_i \phi_i = 0$ without loss of generality. Those eigenstates characterized by the integer m will be called m -symmetric hereafter.

For the ground state, $m = 0$ ($N/2$) for N =odd (even) and the quantization condition (3.1) becomes

$$\phi_i = \sum_j \arg(\Gamma(1 + i(k_i - k_j))) = 0 \pmod{\pi/2} \pmod{\pi} \tag{3.2}$$

for $N = \text{odd}$ (even). Defining the density $\rho(k)$ of k_i s as $N\rho(k_i) = 1/(k_{i+1} - k_i)$, assuming that k_i s will condensate as $N \rightarrow \infty$ and fill continuously an interval $[-Q, Q]$, taking into account $\phi_{i+1} - \phi_i = \pi$, one can obtain the integral equation

$$\rho(x) = \int_{-Q}^Q \frac{dy}{2\pi} K(x - y)\rho(y) \tag{3.3}$$

with $\int_{-Q}^Q \rho(x) dx = 1$, where $K(x - y) = 2\Re\psi(1 + i(x - y))$ and $\psi(z)$ is the digamma function, i.e. $\psi(z) = \Gamma'(z)/\Gamma(z)$. The maximum pseudo-momentum Q turns out as $Q \simeq 2.8992$ [12]

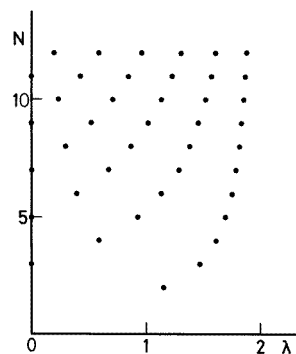


Figure 1. Distributions of $\{\lambda_i\}$ for $2 \leq N \leq 12$ in the case of $D = 0.948$. Only non-negative $\{\lambda_i\}$ are shown since the distribution is symmetric.

The quantization condition of the open lattice in a box in the thermodynamic limit can also be given by a similar argument. Let us set the scale $\hbar = 1$ for simplicity. Then the quantization condition (2.18) becomes

$$\phi_j = \frac{1}{2}L\lambda_j + \sum_k \arg(\Gamma(1 + i(\lambda_j - \varepsilon_k))) - \arg(r_{i\lambda_j}) = \frac{m\pi}{N} \pmod{\pi}. \quad (3.4)$$

Since $r_{i\lambda_j} = 1 + O(e^{-\alpha N})$ and $i\lambda_j = i\varepsilon_j + O(e^{-\beta N})$, equation (3.4) can be further reduced to

$$\phi_i = \frac{1}{2}Lk_i + \sum_j \arg(\Gamma(1 + i(k_i - k_j))) = \frac{m\pi}{N} \pmod{\pi}. \quad (3.5)$$

One should note that (3.5) is exactly the same as the Bethe ansatz equation. Therefore the Bethe ansatz equation gives the exact spectra in the thermodynamic limit. Repeating the argument similar to that of the periodic lattice, one can obtain the integral equation of the density distribution $\rho(k)$ for the ground state

$$\rho(x) = \frac{1}{2\pi} + \int_{-Q}^Q \frac{dy}{2\pi} K(x-y)\rho(y) \quad (3.6)$$

and the density $D = N/L$ is given by

$$D = N/L = \int_{-Q}^Q \rho(x) dx. \quad (3.7)$$

We have solved (3.4) for $2 \leq N \leq 12$ and the integral equation (3.6) for the densities $D = 10.61, 0.948$ and 0.288 , which correspond to the maximum pseudo-momenta $Q = 2.8, 2.0$ and 1.0 , respectively. For example, we show in figure 1 the distributions of $\{\lambda_i\}$ for $2 \leq N \leq 12$ in the case of $D = 0.948$. They tend to distribute outer region as N increases and its upper bound is $Q = 2.0$ ($N \rightarrow \infty$). The numerical factors α, β turned out as $\alpha \simeq 2.30, 2.87, 4.76$ and $\beta \simeq 1.77, 2.25, 3.68$ for $Q = 2.8, 2.0$ and 1.0 , respectively. Combining the result of the periodic lattice which corresponds to $D = \infty$ ($L = 0$), one can obtain the empirical relations

$$\alpha \simeq 0.68/D + 2.2 \quad (3.8)$$

$$\beta \simeq 0.54/D + 1.7. \quad (3.9)$$

3.2. Excited states and Yang–Yang formulation

Yang and Yang [8] developed the thermodynamics of the repulsive δ -function interaction Bose gas based on the Bethe ansatz equation. We will closely follow the idea of Yang and Yang in order to formulate the thermodynamics of the periodic Toda lattice.

For the eigenstate which has an m -symmetry and quantum numbers $\{n_i\}$, we will make equally spaced lattice sites $\{\theta_m, \theta_m \pm \pi, \theta_m \pm 2\pi, \dots\}$ with $\theta_m = m\pi/N$ ($-\pi/2 < \theta_m \leq \pi/2$). The quantum numbers $\{n_i\}$ uniquely determine the angles $\{\phi_i\}$ ($\sum_i \phi_i = 0$) and the pseudo-momenta $\{k_i\}$ according to (3.1). For example, the ground state has the quantum numbers $n_1 = n_2 = \dots = n_{N-1} = 0$ and ϕ_i s are closely packed, thus the pseudo-momenta $\{k_i\}$ fill continuously an interval $[-Q, Q]$ at the large N limit. However, for excited states, there are omitted sites called holes and the range of the pseudo-momentum is not limited.

Let us define the function $\phi(x)$ such that

$$\phi(x) = \sum_j \arg(\Gamma(1 + i(x - k_j))). \tag{3.10}$$

$\phi(x)$ is a monotonically increasing function and $\phi(k_i) = \phi_i$. In the large N limit, we will define the density distributions $\rho(k)$ and $\rho_h(k)$ according to Yang and Yang as follows:

$$N\rho(k) dk = \text{Number of pseudo-momenta in } dk \tag{3.11}$$

$$N\rho_h(k) dk = \text{Number of holes in } dk. \tag{3.12}$$

Defining the function $h(k)$ as $\phi(k) = Nh(k)$ and counting the number of pseudo-momenta and holes in the interval dk , which is equal to the range of $\phi(k)/\pi$ by definition, one can obtain

$$\frac{1}{\pi} d\phi = \frac{1}{\pi} N dh = N(\rho(k) + \rho_h(k)) dk \tag{3.13}$$

$$\frac{dh}{dk} = \pi(\rho(k) + \rho_h(k)). \tag{3.14}$$

In the large N limit, (3.10) becomes

$$h(x) = \int_{-\infty}^{\infty} \arg(\Gamma(1 + i(x - y)))\rho(y) dy \tag{3.15}$$

and its differentiation gives

$$2\pi(\rho(x) + \rho_h(x)) = \int_{-\infty}^{\infty} K(x - y)\rho(y) dy \tag{3.16}$$

where the kernel $K(x - y)$ is the same as (3.3) and the normalization is $\int_{-\infty}^{\infty} \rho(x) dx = 1$. Equation (3.15) is independent of the symmetry, in other words, the way to approach the continuum $\phi_i \rightarrow \phi(x)$ is the same for all m -symmetric states. It is natural since we cannot distinguish the symmetry of each state in thermodynamics.

Let us calculate the partition function Z . Z is defined by

$$Z(\beta) = \sum_{\{n_i\}} \exp(-\beta E[\{n_i\}]) \tag{3.17}$$

where $\beta = 1/T$, putting the Boltzmann constant $k_B = 1$. $E[\{n_i\}]$ is the energy of the state specified by quantum numbers $\{n_i\}$ and the sum is taken over all the possible finite number excitations. One of the important properties of the Toda lattice is that two states which have quantum numbers $\{n_i\} = (n_1, n_2, \dots, n_{N-1})$ and its inverse, i.e. $\{n_i\}_{inv} = (n_{N-1}, n_{N-2}, \dots, n_2, n_1)$, are degenerate [16]:

$$E[\{n_i\}] = E[\{n_i\}_{inv}]. \tag{3.18}$$

For the higher-order conserved quantities A_i , it was also shown [16] that

$$A_i[\{n_i\}] = A_i[\{n_i\}_{inv}] \quad \text{for } i = \text{even} \tag{3.19}$$

$$A_i[\{n_i\}] = -A_i[\{n_i\}_{inv}] \quad \text{for } i = \text{odd}. \tag{3.20}$$

Therefore the eigenvalues of the operator \hat{A}_i ($i = \text{odd}$) come out either in pairs $\pm A_i$ or $A_i = 0$, and their thermodynamic average is identically zero. The pseudo-momenta of the degenerate state are

$$\{k_i\}_{inv} = \{-k_{N+1-i}\} = (-k_N, -k_{N-1}, \dots, -k_2, -k_1). \quad (3.21)$$

The simultaneous eigenvalues A_i s ($i = \text{even}$) can be expressed in terms of the pseudo-momenta $\{k_i\}$ as follows [12, 16]:

$$\sum_{k=0}^{[N/2]} A_{2k} x^{N-2k} = \prod_{i=1}^N (x - k_i) = \prod_{i=1}^N (x + k_i). \quad (3.22)$$

Taking the logarithm of (3.22), dividing by N and taking the continuum limit, one can get

$$\begin{aligned} \ln x + \lim_{N \rightarrow \infty} \frac{1}{N} \ln(1 + A_2 x^{-2} + A_4 x^{-4} + \dots) &= \int_{-\infty}^{\infty} \ln(x - y) \rho(y) dy \\ &= \int_{-\infty}^{\infty} \ln(x - y) \rho_{inv}(y) dy. \end{aligned} \quad (3.23)$$

Since $\rho_{inv}(k) = \rho(-k)$, we have

$$\int_{-\infty}^{\infty} \ln(x - y) \rho_{sym}(y) dy = \ln x + \lim_{N \rightarrow \infty} \frac{1}{N} \ln(1 + A_2 x^{-2} + A_4 x^{-4} + \dots) \quad (3.24)$$

where $\rho_{sym}(y) = \frac{1}{2}(\rho(y) + \rho(-y))$ and it is an even function. Therefore we can assume that the density distribution $\rho(x)$ is an even function, without loss of generality.

By expanding both sides of (3.24) in powers of x at $x \rightarrow \infty$ and comparing the coefficients, the first three terms are

$$\begin{aligned} -\frac{1}{2} \langle \varepsilon^2 \rangle &= \lim_{N \rightarrow \infty} \frac{1}{N} A_2 \\ -\frac{1}{4} \langle \varepsilon^4 \rangle &= \lim_{N \rightarrow \infty} \frac{1}{N} (A_4 - \frac{1}{2} A_2^2) \\ -\frac{1}{6} \langle \varepsilon^6 \rangle &= \lim_{N \rightarrow \infty} \frac{1}{N} (A_6 - A_4 A_2 + \frac{1}{3} A_2^3) \end{aligned} \quad (3.25)$$

where $\langle \varepsilon^n \rangle = \int_{-\infty}^{\infty} x^n \rho(x) dx$. Since the conserved quantities A_{2k} diverge as $O(N^k)$ for $N \rightarrow \infty$, let us expand the divergent part of A_{2k} as

$$A_{2k} \approx a_{2k,k} N^k + a_{2k,k-1} N^{k-1} + \dots + a_{2k,1} N. \quad (3.26)$$

Inserting (3.26) into (3.25) and comparing the N^{l-1} th ($1 \leq l \leq k$) order, one can get the following relations for $k \leq 3$:

$$\begin{aligned} a_{2,1} &= -\frac{1}{2} \langle \varepsilon^2 \rangle & a_{4,1} &= -\frac{1}{4} \langle \varepsilon^4 \rangle & a_{4,2} &= \frac{1}{2} a_{2,1}^2 = \frac{1}{8} \langle \varepsilon^2 \rangle^2 \\ a_{6,1} &= -\frac{1}{6} \langle \varepsilon^6 \rangle & a_{6,2} &= a_{4,1} a_{2,1} = \frac{1}{8} \langle \varepsilon^4 \rangle \langle \varepsilon^2 \rangle \\ a_{6,3} &= a_{4,2} a_{2,1} - \frac{1}{3} a_{2,1}^3 = -\frac{1}{48} \langle \varepsilon^2 \rangle^3. \end{aligned} \quad (3.27)$$

The average energy u per particle is

$$\begin{aligned} u &= E/N = -A_2/N \\ &= -a_{2,1} = \frac{1}{2} \langle \varepsilon^2 \rangle \\ &= \frac{1}{2} \int_{-\infty}^{\infty} x^2 \rho(x) dx. \end{aligned} \quad (3.28)$$

From (3.25)–(3.27) one can show by induction that the leading term of (3.26) can be expressed in terms of the energy:

$$A_{2k} \approx (-1)^k \frac{E^k}{k!}. \tag{3.29}$$

The derivation of (3.29) is rather involved and is postponed to the appendix.

Next we will count the number of states dW for a fixed interval dk according to Yang and Yang,

$$dW = \frac{[N(\rho + \rho_h) dx]!}{[N\rho dx]![N\rho_h dx]!}. \tag{3.30}$$

The entropy dS of this interval is

$$\begin{aligned} dS &= \ln dW \\ &= N(\rho + \rho_h) dx \ln(\rho + \rho_h) - N\rho dx \ln \rho - N\rho_h dx \ln \rho_h \end{aligned} \tag{3.31}$$

and the entropy S is

$$S/N = \int_{-\infty}^{\infty} dx [(\rho + \rho_h) \ln(\rho + \rho_h) - \rho \ln \rho - \rho_h \ln \rho_h]. \tag{3.32}$$

This entropy S corresponds to the whole number of states given by the density distributions ρ and ρ_h , and the symmetry of each state is not specified. In other words, the sum is taken over all possible m -symmetries. Since the symmetry of the state is determined by the whole sequence of filled sites (particles) and omitted sites (holes), the products of the number of states dW contain all symmetries. If one selects one sequence of particles and holes from each interval dk and combines them to make a whole sequence, it belongs to a certain definite m -symmetric state. However, one should sum all possible symmetries afterwards, and it is equivalent to that the symmetry is not specified from the beginning.

In the large N limit, the partition function Z (3.17) can be rewritten by the functional integral of ρ ,

$$\begin{aligned} Z(\beta) &= \int D\rho \exp(-\beta E[\rho] + S[\rho]) \\ &= \int D\rho \exp(-\beta F[\rho]) \end{aligned} \tag{3.33}$$

where $F = E - TS$ is the free energy and its explicit form is

$$F[\rho]/N = \frac{1}{2} \int_{-\infty}^{\infty} dx x^2 \rho - T \int_{-\infty}^{\infty} dx [(\rho + \rho_h) \ln(\rho + \rho_h) - \rho \ln \rho - \rho_h \ln \rho_h]. \tag{3.34}$$

By employing the variational principle, we will approximate the functional integral (3.33) by its maximum contribution which corresponds to an equilibrium. Taking into account the normalization $\int_{-\infty}^{\infty} \rho dx = 1$, the variational equation is

$$\delta F/N - f \delta \int_{-\infty}^{\infty} \rho dx = 0 \tag{3.35}$$

where f is a Lagrange multiplier. Since ρ and ρ_h are related by (3.16), one can get

$$-f + \frac{1}{2}x^2 + T \ln \frac{\rho}{\rho_h} - T \int_{-\infty}^{\infty} \frac{dy}{2\pi} K(x - y) \ln \left(1 + \frac{\rho}{\rho_h} \right) = 0. \tag{3.36}$$

Defining the function $\varepsilon(x)$ such that

$$\frac{\rho_h(x)}{\rho(x)} = \exp(\varepsilon(x)/T) \tag{3.37}$$

we have

$$\varepsilon(x) = -f + \frac{1}{2}x^2 - T \int_{-\infty}^{\infty} \frac{dy}{2\pi} K(x - y) \ln(1 + \exp(-\varepsilon(y)/T)) \quad (3.38)$$

and (3.16) becomes

$$\rho(x)\{1 + \exp(\varepsilon(x)/T)\} = \int_{-\infty}^{\infty} \frac{dy}{2\pi} K(x - y)\rho(y). \quad (3.39)$$

Equations (3.38) and (3.39) are very similar to those of Yang and Yang. However, (3.39) is a homogeneous integral equation, while that of Yang and Yang is inhomogeneous. This difference comes from the fact that the periodic Toda lattice is a closed system having only bound states, while the repulsive δ -interaction gas is an open system having only scattering states. The Lagrange multiplier f has the physical meaning of the free energy per particle in the equilibrium, which contrasts the case of the δ -interaction gas where f is a chemical potential. This is again due to the difference between a closed system and an open system.

Repeating the same argument of Yang and Yang, one can show that the functions $h(k)$ and $\varepsilon_0(k) = \varepsilon(k) + f$ are the momentum and the energy of an elementary excitation, respectively. Since we are studying in the centre-of-mass system, the total momentum is $P = 0$, which naturally results in $\sum_i \phi(k_i) = 0$. On the other hand, the energy difference of the excitation $\{k_\alpha\} \rightarrow \{k'_\alpha\}$ is given by

$$\Delta E = \sum_{\alpha} (\varepsilon_0(k'_\alpha) - \varepsilon_0(k_\alpha)). \quad (3.40)$$

Thermodynamic averages of the higher-order conserved quantities are calculated as follows. From (3.29), $A_{2k}[\rho]$ can be expressed in terms of $E[\rho]$ at $N \rightarrow \infty$:

$$A_{2k}[\rho] = (-1)^k \frac{E[\rho]^k}{k!}. \quad (3.41)$$

Then the thermodynamic average is

$$\langle A_{2k} \rangle = Z^{-1} \frac{(-1)^k}{k!} \int D\rho E[\rho]^k \exp(-\beta F[\rho]). \quad (3.42)$$

We can approximate this functional integral by the same function which satisfies the extremum condition (3.35) within the order $O(\frac{k}{N} \ln N)$. Therefore once the density distribution $\rho(k)$ of the equilibrium and the average energy $\langle E \rangle$ are calculated, then the thermodynamic averages of the higher-order conserved quantities are simply given by $\langle A_{2k} \rangle = \frac{(-1)^k}{k!} \langle E \rangle^k$. These are the same conclusions as the classical Toda lattice [18].

Thermodynamics of the open lattice in a box can also be formulated according to the Yang–Yang method. We will simply write down the resulting integral equations which should replace equations (3.38) and (3.39),

$$\varepsilon(x) = -\mu + \frac{1}{2}x^2 - T \int_{-\infty}^{\infty} \frac{dy}{2\pi} K(x - y) \ln(1 + \exp(-\varepsilon(y)/T)) \quad (3.43)$$

$$\rho(x)\{1 + \exp(\varepsilon(x)/T)\} = \frac{1}{2\pi} + \int_{-\infty}^{\infty} \frac{dy}{2\pi} K(x - y)\rho(y). \quad (3.44)$$

and the density distribution $\rho(x)$ is normalized as $\int_{-\infty}^{\infty} \rho(x) dx = N/L = D$. μ is a chemical potential which is determined by the density D and one should note that (3.44) is an inhomogeneous integral equation which contrasts with the homogeneous equation (3.39).

4. Numerical methods

We have solved coupled integral equations (3.38) and (3.39) of the periodic lattice for $T = 0$ and $T > 0$ and obtained the density distribution $\rho(k)$ and quasi-particle energy $\varepsilon(k)$. In this section, we will describe the numerical method in some detail. Numerical results will be discussed in the next section. The calculation of the open lattice in a box has been carried out by Hader and Mertens [7] and we will refer to their results.

4.1. $T = 0$

Let us assume that the quasi-particle energy $\varepsilon(k)$ is a monotonically increasing function of k^2 and has a zero at $k^2 = Q^2$. This behaviour is the same as the δ -interaction gas and this assumption will be confirmed by the numerical calculation. Then (3.38) and (3.39) are simplified as

$$\varepsilon(x) = -f + \frac{1}{2}x^2 + \int_{-Q}^Q \frac{dy}{2\pi} K(x-y)\varepsilon(y) \tag{4.1}$$

$$\rho(x) = \int_{-Q}^Q \frac{dy}{2\pi} K(x-y)\rho(y). \tag{4.2}$$

Equation (4.2) is the same as equation (3.3). For $|k| > Q$, $\rho(k) = 0$. In the case of $T = 0$, equations for $\varepsilon(k)$ and $\rho(k)$ are decoupled and they are solved separately.

Equation (4.2) is a homogeneous Fredholm equation of the second kind. The kernel is $K(x-y) = 2\Re\psi(1+i(x-y))$ and

$$\Re\psi(1+iu) = -\gamma_E + u^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2+u^2)} \quad (|u| < \infty) \tag{4.3}$$

where $\gamma_E = 0.5772\dots$ is Euler's constant. Since the kernel is free from singularities, it can be numerically solved easily. For example, we have solved (4.2) either by employing the Gauss-Legendre quadratures and discretizing the equation, or by expanding the kernel in terms of orthogonal functions in [12]. It is a kind of eigenvalue problem, i.e. one should search an eigenvalue Q such that there exists an eigenfunction $\rho(k)$.

Equation (4.1) is an inhomogeneous Fredholm equation of the second kind. Since (4.2) indicates that one of the eigenvalues of the kernel is unity, we cannot solve (4.1) by discretization and matrix inversion. Let us denote the eigenvalues and the eigenfunctions of the kernel $\frac{1}{2\pi}K(x-y)$ by $\{\lambda_i\}$ and $\{\varphi_i\}$,

$$\int_{-Q}^Q \frac{dy}{2\pi} K(x-y)\varphi_i(y) = \lambda_i\varphi_i(x) \tag{4.4}$$

and assign $\lambda_0 = 1$, $\varphi_0(x) \propto \rho(x)$. Eigenfunctions are assumed to be normalized as $\int_{-Q}^Q dx \varphi_i(x)\varphi_j(x) = \delta_{ij}$. Let us expand the inhomogeneous term $\varepsilon_1(x) = -f + \frac{1}{2}x^2$ and the solution $\varepsilon(x)$ in terms of the eigenfunctions $\{\varphi_i\}$. By substituting these expansions into (4.1) and comparing the coefficients, one can obtain

$$\varepsilon(x) = \varepsilon_1(x) + c_0\rho(x) + \sum_{n \geq 1} \frac{\varepsilon_n \lambda_n}{1 - \lambda_n} \varphi_n(x) \tag{4.5}$$

where $\varepsilon_n = \int_{-Q}^Q dx \varepsilon_1(x)\varphi_n(x)$. The coefficient c_0 is indefinite and it is determined by the condition $\varepsilon(\pm Q) = 0$.

4.2. $T > 0$

For finite temperature $T > 0$, equations (3.38) and (3.39) are coupled and we must solve them consistently. Let us rewrite (3.39) in a symmetric way:

$$\rho_s(x) = \int_{-\infty}^{\infty} \frac{dy}{2\pi} K_s(x-y)\rho_s(y) \quad (4.6)$$

where

$$K_s(x-y) = [1 + \exp(\varepsilon(x)/T)]^{-1/2} K(x-y) [1 + \exp(\varepsilon(y)/T)]^{-1/2} \quad (4.7)$$

$$\rho_s(x) = [1 + \exp(\varepsilon(x)/T)]^{1/2} \rho(x). \quad (4.8)$$

First we will solve (3.38) by iteration by starting with the inhomogeneous term $\varepsilon_1(x) = -f + \frac{1}{2}x^2$ with a certain initial value f . Once $\varepsilon(x)$ is calculated, next we calculate the eigenvalues of the kernel $\frac{1}{2\pi} K_s(x-y)$. Equation (4.6) indicates that one of the eigenvalues of the kernel $\frac{1}{2\pi} K_s(x-y)$ is unity and its eigenfunction is $\rho_s(x)$. Therefore, if none of the eigenvalues are unity, we solve (3.38) with a different initial value f and repeat the above process until the kernel $\frac{1}{2\pi} K_s(x-y)$ has an eigenvalue 1. In practical calculation, the largest eigenvalue is well separated from others, and it is not so difficult to find the value f such that the kernel has an eigenvalue 1. We have mapped $(-\infty, \infty)$ to a finite interval and employed Gauss–Legendre quadratures. In the low temperature region, the density distribution $\rho(x)$ varies rapidly around $x = q$ satisfying $\varepsilon(q) = 0$ and many mesh points are distributed around $x = q$. In solving (3.38), we have used another technique [7]. Since the kernel $K(x-y)$ diverges at $|x-y| \rightarrow \infty$, i.e. $K(x-y) \sim \ln|x-y|$, we made the kernel finite by subtracting $\varepsilon(0)$,

$$\varepsilon(0) = -f - T \int_{-\infty}^{\infty} \frac{dy}{2\pi} K(y) \ln(1 + \exp(-\varepsilon(y)/T)). \quad (4.9)$$

Subtraction (4.9) from (3.38) gives

$$\varepsilon(x) = \varepsilon(0) + \frac{1}{2}x^2 - T \int_{-\infty}^{\infty} \frac{dy}{2\pi} K_1(x-y) \ln(1 + \exp(-\varepsilon(y)/T)) \quad (4.10)$$

where $K_1(x-y) = K(x-y) - K(y)$ and $K_1(x-y) \rightarrow 0$ at $|y| \rightarrow \infty$. Therefore, in practice, we have solved (4.10) with a certain initial value $\varepsilon(0)$. Once consistent solutions $\varepsilon(x)$, $\varepsilon(0)$ and $\rho(x)$ are obtained, the free energy f per particle is given by

$$f = -\varepsilon(0) - T \int_{-\infty}^{\infty} \frac{dy}{2\pi} K(y) \ln(1 + \exp(-\varepsilon(y)/T)). \quad (4.11)$$

5. Results and discussion

In figure 2, we show the density distributions $\rho(k)$ of the pseudo-momentum for $T = 0, 0.2, 0.5, 1$ and 2 . The maximum pseudo-momentum at $T = 0$ is $Q \simeq 2.8992$. This is similar to a free Fermi gas and Q is called pseudo Fermi momentum. The density is larger for large k value. This behaviour is quite different from other completely integrable models. For example, density distributions of the δ -interaction Bose gas [3] and Calogero–Sutherland model [4] have a maximum at $k = 0$ and they monotonically decrease in the larger k -region. In the classical limit $\hbar \rightarrow 0$, Sutherland [5] has shown that the density distribution is given by

$$\rho(k) = \frac{1}{\pi(Q^2 - k^2)^{1/2}}. \quad (5.1)$$

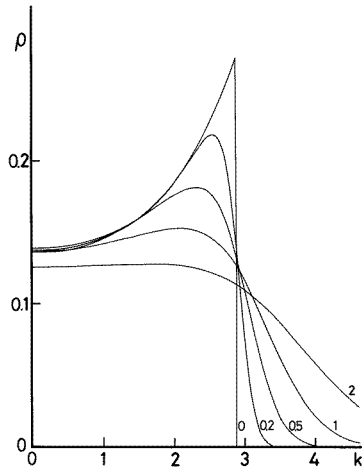


Figure 2. Density distributions $\rho(k)$ of the pseudo-momentum for $T = 0, 0.2, 0.5, 1$ and 2 .

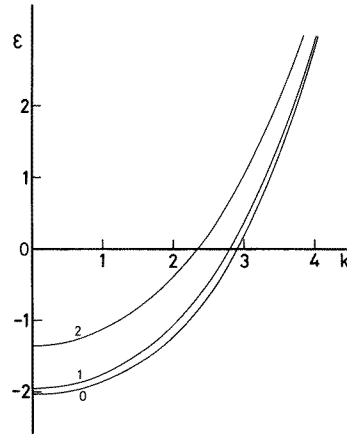


Figure 3. Quasi-particle energies $\varepsilon(k)$ for $T = 0, 1$ and 2 .

It diverges at the maximum $|k| = Q$, however, figure 2 shows that the exact $\rho(k)$ remains finite at $|k| = Q$.

At low temperature $T \simeq 0$, the density slightly diffuses and its behaviour around $|k| \simeq Q$ is approximately given by

$$\rho(k, T) \simeq [1 + \exp(\varepsilon(k)/T)]^{-1} \rho(Q, T = 0) + O(T^2). \quad (5.2)$$

This is also similar to a free Fermi gas. As the temperature T increases, particle-hole excitations increase near the Fermi level.

In figure 3, we show the quasi-particle energies $\varepsilon(k)$ for $T = 0, 1$ and 2 . In the classical limit, Sutherland also showed that

$$\varepsilon(k) = -(Q^2 - k^2)^{1/2} \quad (|k| < Q) \quad (5.3)$$

and our exact calculation exhibits similar behaviour. This behaviour is similar to that of the δ -interaction Bose gas. Although we do not prove in a mathematically rigorous way that $\varepsilon(k)$ is a monotonically increasing function of k^2 , our numerical calculation certainly indicates that our assumption is correct.

We show in figure 4 the temperature dependence of the free energy $f(T)$ per particle. At $T = 0$, $f(0) \simeq 1.6762$, which is the average energy per particle of the ground state. $f(T)$ is a monotonically decreasing function of T .

We show the average energy $u(T)$ and the specific heat $C(T)$ per particle in figures 5 and 6, respectively. $C(0) = 0$ and it rapidly increases for $T > 0$, then it gradually decreases after reaching its maximum $C \simeq 0.84$ at $T \simeq 2$. In order to make a comparison, we also plotted the classical values $u_{cl}(T)$ and $C_{cl}(T)$ [18, 19]. At $T \rightarrow \infty$, the system behaves like a classical one, and $u(T) \sim u_{cl}(T) \rightarrow T/2$, $C(T) \sim C_{cl}(T) \rightarrow \frac{1}{2}$. If the exponential potential is truncated by the second order, i.e. $e^x \simeq 1 + x + \frac{1}{2}x^2$, the Toda lattice is reduced to the harmonic chain (hc). The Hamiltonian of the harmonic chain can be expressed as a sum of harmonic oscillators and their eigenvalues are easily obtained. The average energy $u_{hc}(T)$ and the specific heat $C_{hc}(T)$ of the harmonic chain are given by

$$u_{hc}(T) = 1 + \int_0^1 dx \coth(\beta \sin \pi x) \sin \pi x \quad (5.4)$$

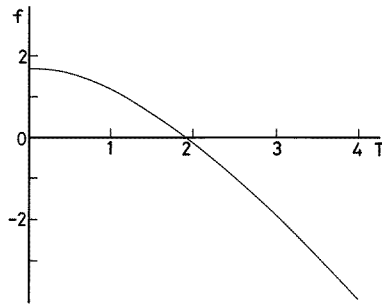


Figure 4. Free energy $f(T)$ per particle versus T .

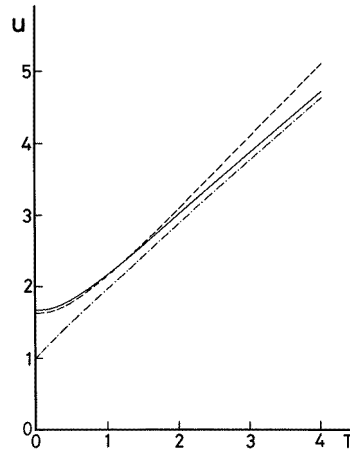


Figure 5. Average energy $u(T)$ per particle versus T (full curve). Average energies of the classical system and the harmonic chain are also shown by chain and broken curves, respectively.

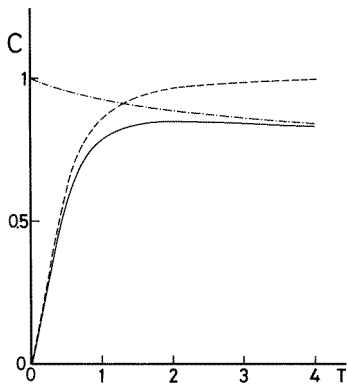


Figure 6. Specific heat $C(T)$ per particle versus T (full curve). Specific heats of the classical system and the harmonic chain are also shown by chain and broken curves, respectively.

$$C_{hc}(T) = \beta^2 \int_0^1 dx \sinh^{-2}(\beta \sin \pi x) \sin^2 \pi x. \quad (5.5)$$

$u_{hc}(T)$ and $C_{hc}(T)$ are also plotted in figures 5 and 6. At $T = 0$, $u_{hc}(0) = 1 + 2/\pi \simeq 1.6366$, which is less than that of the Toda lattice. However, it exceeds the value of the Toda lattice as T increases. It is due to the fact that the harmonic chain is more easily excited than the Toda lattice. This behaviour is more evident in the specific heat. At $T \rightarrow 0$, $C_{hc}(T) \simeq \frac{\pi}{3}T \simeq 1.047T$, while $C_{Toda}(T) \simeq \gamma T$ with $\gamma = \frac{2\pi^2 \rho(Q)}{3e'(Q)} \simeq 0.9728$. When $T \rightarrow \infty$, $C_{hc}(T) \rightarrow 1$ while $C_{Toda}(T) \rightarrow 1/2$.

Our results are similar to those of the open Toda lattice in a box [6, 7]. It is understandable since bulk properties do not depend on the way of confining the system.

6. Summary

We have studied the thermodynamics of the periodic Toda lattice based on Gutzwiller's quantization condition and Yang and Yang's formulation. Although the basic equations (3.38) and (3.39) look quite similar to those of Yang and Yang's equations,

(3.39) is a homogeneous equation while that of Yang and Yang for the repulsive δ -function interaction gas is inhomogeneous. This difference comes from the fact that the periodic Toda lattice is a closed system having only bound states and, in contrast, the repulsive δ -interaction gas is an open system having only scattering states. In the case of the open Toda lattice in a box, Gutzwiller's quantization condition becomes identical to the Bethe ansatz equation in the thermodynamic limit. Yang and Yang's equation of the open lattice becomes the same inhomogeneous type as the repulsive δ -function interaction gas.

We have solved equations (3.38) and (3.39) and obtained the density distribution $\rho(k)$ of the pseudo-momentum and the energy $\varepsilon(k)$ of the quasi-particle. The density distribution $\rho(k)$ is quite different from other integrable models, i.e. $\rho(k)$ increases in the larger k -region. However, except for this characteristic behaviour, other properties are quite similar to those of a free Fermi gas. This similarity is also true for the quasi-particle energy $\varepsilon(k)$. Making use of the density $\rho(k)$, we have calculated the average energy $u(T)$ and the specific heat $C(T)$ per particle for the temperature range $0 \leq T \leq 4$. We have also calculated the thermodynamic averages of the higher-order conserved quantities and it turns out that they are expressed in terms of the average energy $\langle E \rangle$ as $\langle A_{2k} \rangle = \frac{(-1)^k}{k!} \langle E \rangle^k$, which is the same as the classical Toda lattice. In the high temperature limit $T \rightarrow \infty$, $u(T)$ and $C(T)$ certainly become close to those of the classical system. On the other hand, in the low temperature region, it behaves like a harmonic chain. These are due to the characteristics of the Toda lattice which behaves like either a hard-sphere gas or a harmonic chain in opposite limiting cases.

Appendix

In this appendix, we will prove (3.29). Let us define the function $F(x)$ such that

$$F(x) = \sum_{m=1}^{\infty} A_{2m} x^{-2m}. \tag{A1}$$

Then the expansion of the RHS of (3.24) in powers of x at $x \rightarrow \infty$ is

$$\ln(1 + F(x)) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{1}{n} F(x)^n \tag{A2}$$

and we will write $F(x)^n$ as

$$F(x)^n = \left(\sum_{m=1}^{\infty} A_{2m} x^{-2m} \right)^n = \sum_{m=1}^{\infty} c_{m,n} x^{-2m}. \tag{A3}$$

The coefficients $c_{m,n}$ satisfy the following recursion relation:

$$c_{m,n} = c_{m-1,n-1} A_2 + c_{m-2,n-1} A_4 + \dots + c_{n-1,n-1} A_{2m-2n+2} \quad (2 \leq n \leq m). \tag{A4}$$

Let us assume that the leading term of A_{2j} is

$$A_{2j} \approx (-1)^j \frac{E^j}{j!} = \frac{(-u)^j}{j!} N^j \tag{A5}$$

for $j \leq k - 1$ and employ an induction to prove that (A.5) is also valid for $j = k$.

From the recursion relation (A4) and the initial value $c_{m,1} = A_{2m}$ ($m \leq k - 1$), one can show by the induction of the index n that the coefficient $c_{m,n}$ can be given by

$$c_{m,n} = \frac{(-u)^m N^m}{m!} \{ {}_n C_0 n^m - {}_n C_1 (n-1)^m + {}_n C_2 (n-2)^m + \dots + (-1)^n {}_n C_{n-2} 2^m + (-1)^{n-1} {}_n C_{n-1} \} \quad (2 \leq n \leq m \leq k). \tag{A6}$$

The proof is rather tedious but straightforward by employing properties of binomial coefficients.

Since the LHS of (3.24) is finite, the order of (A2) is $O(N)$ and the coefficient of $O(N^k)$ ($k \geq 2$) should vanish, which results in the following equations:

$$c_{k,1} - \frac{1}{2}c_{k,2} + \frac{1}{3}c_{k,3} - \cdots + (-1)^{k-1} \frac{1}{k}c_{k,k} = 0 \quad (\text{A7})$$

and

$$c_{k,1} = \sum_{\ell=2}^k (-1)^\ell \frac{1}{\ell} c_{k,\ell} = \frac{(-u)^k N^k}{k!} \sum_{\ell=2}^k (-1)^\ell \frac{1}{\ell} \{ {}_\ell C_0 \ell^k - {}_\ell C_1 (\ell-1)^k + {}_\ell C_2 (\ell-2)^k + \cdots + (-1)^\ell {}_\ell C_{\ell-2} 2^k + (-1)^{\ell-1} {}_\ell C_{\ell-1} \}. \quad (\text{A8})$$

Using the explicit formula (A6), one can derive

$$\begin{aligned} c_{k,1} &= \frac{(-u)^k N^k}{k!} \left\{ \sum_{n=0}^{k-1} (-1)^{k-n} (k-n)^{k-1} \frac{1}{n!} k(k-1)(k-2)\cdots(k-n+1) + 1 \right\} \\ &= \frac{(-u)^k N^k}{k!} \left\{ \sum_{n=1}^k (-1)^n n^{k-1} {}_k C_n + 1 \right\} \\ &= \frac{(-u)^k N^k}{k!}. \end{aligned} \quad (\text{A9})$$

since $\sum_{n=1}^k (-1)^n n^{k-1} {}_k C_n = 0$. Therefore $A_{2k} = \frac{(-u)^k N^k}{k!}$ is proved.

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