# Ground state of the quantum periodic Toda lattice in the large- *N* limit



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# Ground state of the quantum periodic Toda lattice in the large-$N$ limit

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**Abstract.** In Gutzwiller's formulation of the quantum periodic Toda lattice, quantization conditions are expressed in terms of Floquet's characteristic exponents which are equal to the zeros of a Hill-type determinant. We have derived an integral equation for the density distribution of those zeros for the ground state in the large-$N$ limit. The large-$N$ asymptotic expansions of the conserved quantities given by this density distribution are found to be fairly good approximations to the exact values. We have also carried out the semiclassical quantization by the EBK formulation and the semiclassical eigenvalues turned out to be very close to the exact values.

## 1. Introduction

The Toda lattice is a one-dimensional dynamical system of equal masses connected by nonlinear springs of exponential type between pairs of nearest neighbours [1]. It is one of the most popular models of completely integrable systems [2] and has been studied extensively over two decades. The importance of the Toda lattice consists in its complete integrability, i.e. the classical orbit stays on the invariant torus in the phase space, while the quantum mechanical spectrum and the eigenfunction are characterized by as many quantum numbers as degrees of freedom. There are two kinds of lattices, periodic or open, depending on whether the first and the last masses are coupled or not. In classical mechanics, Flaschka [3] has solved an initial-value problem of the infinite open Toda lattice by the inverse scattering method, while the solution of the periodic Toda lattice is given by the Jacobi inversion method by Kac and Moerbeke [4] and Date and Tanaka [5]. In quantum mechanics, the infinite open Toda lattice was investigated by Sutherland [6] as a limiting case of the $1/\sinh^2(x)$ potential. The quantum version of the periodic Toda lattice was first studied by Gutzwiller [7]. He has developed a formulation which is parallel to the method of [4]. His method is to expand the eigenfunction of the $N$-particle periodic Toda lattice in terms of the product of the $(N-1)$-particle open Toda lattice and a free particle. Meanwhile, Sklyanin [8] 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. The first numerical calculation based on Gutzwiller's formulation was reported by Fowler and Frahm [9], while we have directly carried out the diagonalization of the Hamiltonian in terms of orthogonal bases [10, 11] and similar work was also reported by Isola *et al* [12]. In [11], we have shown that the Hamiltonian has a symmetry of the dihedral group $D_N$ and classified the eigenstates according to the irreducible representations of the $D_N$ group. It is also found that the eigenvalues satisfy Gutzwiller's quantization conditions and the semiclassical quantization is a good approximation.

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The difficulty of the quantum Toda lattice is that no explicit formulae are known for the spectrum and the eigenfunction. This situation contrasts with other well known integrable systems like a Bose gas with $\delta$-function interaction [13] or the Calogero–Sutherland model (CSM) [14]. For example, the eigenfunction of the CSM can be expressed in terms of a Jastrow-type wavefunction which is the product of two-body wavefunctions and its energy spectrum is given by the asymptotic Bethe ansatz. On the other hand, in the case of the Toda lattice, one is forced to carry out numerical calculations which becomes a formidable task for a large number of particles. This is one of the reasons why the quantum Toda lattice has not been studied very much so far. In order to overcome this unsatisfactory situation, we will handle the problem in the opposite direction, i.e. we will firstly solve the problem in the large-$N$ limit and then obtain the exact spectrum of the finite-$N$ system by making use of an asymptotic expansion. The aim of this paper is to derive an integral equation from Gutzwiller's formulation in the large-$N$ limit and show how the exact spectra of the conserved quantities can be practically calculated by employing the solution of this integral equation.

In section 2, we will briefly review Gutzwiller's quantization conditions and, in section 3, an integral equation is derived for the ground state in the large-$N$ limit by employing Gutzwiller's quantization conditions. Semiclassical quantization will be also carried out by the EBK formulation in section 4. Numerical results will be presented in section 5 and section 6 is devoted to a summary.

## 2. Gutzwiller's quantization conditions

The Hamiltonian of the periodic $N$-particle Toda lattice is given in a dimensionless form as

$$H_{\mathrm{Toda}} = \frac{1}{2}\sum_i p_i^2 + \sum_i \exp(q_i - q_{i+1}) \tag{1}$$

where we set $q_{N+1} = q_1$. The classical equations of motion were shown to be rewritten in a Lax form by Flaschka [15]

$$\frac{\mathrm{d}L}{\mathrm{d}t} = [B, L] \tag{2}$$

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

$$L = \begin{pmatrix} b_1 & a_1 & & & & a_N \\ a_1 & b_2 & a_2 & & \text{0} & \\ & \cdots & \cdots & & & \\ & & \cdots & \cdots & & \\ & \text{0} & a_{N-2} & b_{N-1} & a_{N-1} & \\ a_N & & & a_{N-1} & b_N & \end{pmatrix} \tag{3}$$

$$B = \begin{pmatrix} 0 - a_1 & & & & a_N & \\ a_1 & 0 - a_2 & & \text{0} & & \\ & \cdots & \cdots & & & \\ & & \cdots & \cdots & & \\ & \text{0} & a_{N-2} & 0 - a_{N-1} & & \\ -a_N & & & a_{N-1} & 0 & \end{pmatrix} \tag{4}$$

and $a_n = \exp((q_n - q_{n+1})/2)/2$, $b_n = p_n/2$. Therefore the eigenvalues of the matrix $L$ are constants of motion and thus the coefficients of the characteristic polynomial of the matrix

$L$ are also constants of motion, which are defined as follows ($I$ is the $N \times N$ identity matrix),

$$\det(2xI - 2L) = \sum_i A_i (2x)^{N-i} - 2 \tag{5}$$

where $A_0 = 1$. The conserved quantities $A_i$ are in involution with the Hamiltonian, $[H, A_i] = 0$, and also mutually in involution, $[A_i, A_j] = 0$. (Note that $H = -A_2$ in the CM system.) In quantum mechanics, the Hamiltonian and the conserved quantities are operators and are given by the canonical quantization, i.e. the momentum $p_i$ is replaced by the operator $-\mathrm{i}\hbar(\partial/\partial q_i)$. Although the Hamiltonian of the quantum Toda lattice is not scale-invariant, we set $\hbar = 1$ in the following arguments.

In [7], Gutzwiller developed a systematic way of constructing simultaneous eigenfunctions of the operators $H$ and $A_i$ 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 of Pasquier and Gaudin [16]. 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 $H$ and $A_i$.

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

$$C = \begin{pmatrix} \ddots & \ddots & & & & \\ \ddots & 1 & \frac{\pm 1}{D(\kappa-1)} & & \mathbf{0} & \\ & \frac{1}{D(\kappa)} & 1 & \frac{\pm 1}{D(\kappa)} & & \\ & & \frac{1}{D(\kappa+1)} & 1 & \frac{\pm 1}{D(\kappa+1)} & \\ & \mathbf{0} & & \frac{1}{D(\kappa+2)} & 1 & \ddots \\ & & & & \ddots & \ddots \end{pmatrix} \tag{6}$$

where

$$D(\kappa) = \kappa^N + E\kappa^{N-2} - \mathrm{i}A_3\kappa^{N-3} + A_4\kappa^{N-4} + \mathrm{i}A_5\kappa^{N-5} + \cdots + \mathrm{i}^N A_N \tag{7}$$

where $\kappa$ is a complex number and the double sign is $-$ $(+)$ for $N =$ odd (even). It generally has $N$ different purely imaginary solutions $\kappa_i$ $(\sum_i \kappa_i = 0)$ in $-\frac{1}{2} \leqslant \Re(\kappa) \leqslant \frac{1}{2}$. In the special case of $N =$ odd and $A_3 = A_5 = \cdots = 0$, $\Delta(\kappa) = 0$ has $N - 1$ solutions, and $\kappa = 0$ should be added to them since $\kappa = 0$ automatically satisfies the quantization condition. 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

$$\Delta(\mathrm{i}\lambda) = r_{\mathrm{i}\lambda} r^*_{\mathrm{i}\lambda-1} \pm r^*_{\mathrm{i}\lambda} r_{\mathrm{i}\lambda+1} / \{D(\mathrm{i}\lambda) D(\mathrm{i}\lambda + 1)\} \tag{8}$$

where $r_\kappa$ is defined by the recursion relation

$$r_{\kappa-1} = r_\kappa \pm r_{\kappa+1} / \{D(\kappa) D(\kappa + 1)\} \tag{9}$$

with the boundary condition $r_\kappa \to 1$ $(\Re(\kappa) \to \infty)$. The double sign is $+$ $(-)$ for $N =$ odd (even). The solution $r_\kappa$ 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

$$C' = \begin{pmatrix} 1 & \frac{\pm 1}{D(\kappa+1)} & 0 & \\ \frac{1}{D(\kappa+2)} & 1 & \frac{\pm 1}{D(\kappa+2)} & \\ 0 & \frac{1}{D(\kappa+3)} & 1 & \ddots \\ & & \ddots & \ddots \end{pmatrix}. \tag{10}$$

Let $\kappa = \mathrm{i}\lambda_j$ $(\lambda_1 < \lambda_2 < \cdots < \lambda_N)$ be one of the zeros of Hill's determinant, that is, Floquet's characteristic exponent. Then, secondly, Gutzwiller's quantization conditions are expressed as

$$\phi_j = \sum_k \arg\bigl(\Gamma(1 + \mathrm{i}(\lambda_j - \varepsilon_k))\bigr) - \arg(r_{\mathrm{i}\lambda_j}) = \frac{m\pi}{N} \qquad (\mathrm{mod}\ \pi) \tag{11}$$

where $\{\mathrm{i}\varepsilon_k\}$ $(\varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_N)$ are $N$ different zeros of the polynomial $D(\kappa)$ (thus the poles of $\Delta(\kappa)$) and $\phi_j$ is a monotonically increasing function of $\lambda_j$, i.e. $\phi_{j+1} - \phi_j = \pi(n_j + 1)$ with non-negative integers $n_j$ [9]. These $N-1$ non-negative integers $(n_1, n_2, \ldots, n_{N-1})$ 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 $D_N$ group [11]. It takes the values $m = 0, \pm 1, \pm 2, \ldots, \pm(N-1)/2$ for $N =$ odd and $m = 0, \pm 1, \pm 2, \ldots, \pm(N-2)/2, N/2$ for $N =$ even.

Although Gutzwiller's algorithm is well defined, practical calculation is very difficult for a many-body system since one must search simultaneously $N - 1$ eigenvalues $(E, A_3, A_4, \ldots, A_N)$ for given quantum numbers $(n_1, n_2, \ldots, n_{N-1})$. This becomes a formidable task for a large number of particles and another way of calculation should be pursued.

## 3. Ground state in the large-$N$ limit

Let us consider the ground state of the quantum Toda lattice in the large-$N$ limit. The ground state has the quantum numbers $n_1 = n_2 = \cdots = n_{N-1} = 0$ and the integer value $m = 0$ $(N/2)$ for $N =$ odd (even), and it belongs to the irreducible representation of the $A_1$-symmetry (symmetric state) of the $D_N$ group. Therefore the eigenvalues of the conserved quantities $A_n$ $(n =$ odd) vanish since the operators $A_n$ have the $A_2$-symmetry for $n =$ odd (see [11] for details). Also note that the zeros $\mathrm{i}\lambda_j$ and the poles $\mathrm{i}\varepsilon_j$ come out in a symmetric way, i.e. $\lambda_1 = -\lambda_N, \lambda_2 = -\lambda_{N-1}, \ldots, \varepsilon_1 = -\varepsilon_N, \varepsilon_2 = -\varepsilon_{N-1}, \ldots$ $(\lambda_{(N+1)/2} = \varepsilon_{(N+1)/2} = 0$ for $N =$ odd).

In the large-$N$ limit, we will show the following two important properties of Hill's determinant.

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

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

The first one, $r_{\mathrm{i}\lambda_j} = 1 + \mathrm{O}(\mathrm{e}^{-\alpha N})$, can be understood as follows. From the recursion relation (9), one can see

$$r_{\mathrm{i}\lambda} = 1 + \frac{1}{D(\mathrm{i}\lambda + 1)D(\mathrm{i}\lambda + 2)} + \text{(higher order terms)} \tag{12}$$

where higher order terms decrease faster than the second term at $N \to \infty$. Since

$D(\kappa) = \prod_j (\kappa - \mathrm{i}\varepsilon_j)$,

$$|D(\mathrm{i}\lambda + 1)D(\mathrm{i}\lambda + 2)| = \prod_{j=1}^{N} |(\mathrm{i}\lambda - \mathrm{i}\varepsilon_j + 1)(\mathrm{i}\lambda - \mathrm{i}\varepsilon_j + 2)| \approx \Delta_1^N \Delta_2^N \tag{13}$$

where $\ln \Delta_1$ ($\ln \Delta_2$) is the average of $\ln |\mathrm{i}\lambda - \mathrm{i}\varepsilon_j + 1|$ ($\ln |\mathrm{i}\lambda - \mathrm{i}\varepsilon_j + 2|$) and clearly $\Delta_1 > 1$ ($\Delta_2 > 2$). Thus $r_{\mathrm{i}\lambda} \approx 1 + (\Delta_1 \Delta_2)^{-N}$ ($N \to \infty$). Our numerical calculation up to $N = 20$ indicates $\Delta_1 \Delta_2 = 5$–10.

The second one, $\mathrm{i}\lambda_j = \mathrm{i}\varepsilon_j + \mathrm{O}(\mathrm{e}^{-\beta N})$, is a little involved. Hill's determinant $\Delta(\kappa)$ has poles $\{\mathrm{i}\varepsilon_j - n\}$ ($n$ is an integer, $-\infty < n < \infty$ ) and the residue $\mathrm{i}K_j$ at $\kappa = \mathrm{i}\varepsilon_j - n$ can be calculated

$$\begin{aligned} \mathrm{i}K_j &= \lim_{\kappa \to \mathrm{i}\varepsilon_j - n} (\kappa - \mathrm{i}\varepsilon_j + n)\Delta(\kappa) \\ &= \mp(-\mathrm{i})^{N-1} \left\{ \frac{r_{\mathrm{i}\varepsilon_j} r^*_{\mathrm{i}\varepsilon_j+1}}{D(\mathrm{i}\varepsilon_j - 1)} + \frac{r^*_{\mathrm{i}\varepsilon_j} r_{\mathrm{i}\varepsilon_j+1}}{D(\mathrm{i}\varepsilon_j + 1)} \right\} \prod_{k \neq j} (\varepsilon_j - \varepsilon_k)^{-1} \\ &\quad + (\text{higher order terms})\,. \end{aligned} \tag{14}$$

The double sign is $-$ ($+$) for $N =$ odd (even). Since $D(\mathrm{i}\varepsilon_j - 1)^* = (-1)^N D(\mathrm{i}\varepsilon_j + 1)$, $K_j$ is a real number. We know that $r_{\mathrm{i}\varepsilon_j} \approx 1$, $r_{\mathrm{i}\varepsilon_j+1} \approx 1$ and $1/D(\mathrm{i}\varepsilon_j - 1)$ decreases exponentially as $N \to \infty$. However, the behaviour of $\prod_{k \neq j} (\varepsilon_j - \varepsilon_k)^{-1}$ cannot be given by this formula. By making use of the exact calculation, which will be shown in section 5 in detail, it is found that $\varepsilon_j$'s distribute in a finite region and

$$\prod_{k \neq j} (\varepsilon_j - \varepsilon_k) \approx \Delta_3^N \tag{15}$$

with $\Delta_3 = 1.2$–2.0. Thus the residue is $\mathrm{i}K_j \approx \mathrm{O}(\mathrm{e}^{-\beta N})$ ($\beta > 0$) at $N \to \infty$. Since Hill's determinant $\Delta(\kappa)$ has poles $\{\mathrm{i}\varepsilon_j - n\}$ and zeros $\{\mathrm{i}\lambda_j - n\}$, it can be written in a form [16]

$$\Delta(\kappa) = \prod_{k=1}^{N} \frac{\sin \pi(\kappa - \mathrm{i}\lambda_k)}{\sin \pi(\kappa - \mathrm{i}\varepsilon_k)} \tag{16}$$

and the residue at $\kappa = \mathrm{i}\varepsilon_j - n$ is

$$\mathrm{i}K_j = (-1)^n \frac{\prod_{k=1}^{N} \sin \pi(\mathrm{i}\varepsilon_j - \mathrm{i}\lambda_k)}{\pi \prod_{k \neq j}^{N} \sin \pi(\mathrm{i}\varepsilon_j - \mathrm{i}\varepsilon_k)}\,. \tag{17}$$

Since $\mathrm{i}K_j \approx \mathrm{O}(\mathrm{e}^{-\beta N})(N \to \infty)$ and numerical calculation indicates $\lambda_j \approx \varepsilon_j$, one can conclude that $\lim_{N \to \infty} \lambda_j = \varepsilon_j$ and $|K_j| \approx |\varepsilon_j - \lambda_j|$, thus, $\varepsilon_j - \lambda_j = \mathrm{O}(\mathrm{e}^{-\beta N})$.

These two facts, i.e. $r_{\mathrm{i}\lambda_j} = 1 + \mathrm{O}(\mathrm{e}^{-\alpha N})$ and $\mathrm{i}\lambda_j = \mathrm{i}\varepsilon_j + \mathrm{O}(\mathrm{e}^{-\beta N})$ at $N \to \infty$, largely simplify the quantization conditions (11) for the ground state in the large-$N$ limit and it becomes

$$\phi_j = \sum_k \arg\big(\Gamma(1 + \mathrm{i}(\varepsilon_j - \varepsilon_k))\big) = 0 \quad (\pi/2) \quad (\mathrm{mod}\ \pi) \tag{18}$$

for $N =$ odd (even). Defining the density $\rho(\varepsilon)$ of $\varepsilon_j$'s as $N\rho(\varepsilon_j) = 1/(\varepsilon_{j+1} - \varepsilon_j)$, assuming that $\varepsilon_j$'s will condense as $N \to \infty$ and fill continuously an interval $[-Q, Q]$, taking into account the fact that $\phi_{j+1} - \phi_j = \pi$ for the ground state, one can obtain the integral equation in the same way as [6],

$$\frac{1}{\pi} \int_{-Q}^{Q} K(x - y)\rho(y)\,\mathrm{d}y = \rho(x) \tag{19}$$

with $\int_{-Q}^{Q}\rho(x)\,\mathrm{d}x = 1$, where $K(x-y) = \Re\psi(1+\mathrm{i}(x-y))$ and $\psi(z)$ is the digamma function, i.e. $\psi(z) = \Gamma'(z)/\Gamma(z)$. Equation (19) is the same equation derived by Sklyanin under some reasonable assumptions [8]. It is also similar to the Bethe ansatz equation of the open Toda lattice in a box in the thermodynamic limit given by Sutherland [6] and Hader and Mertens [17]. However, equation (19) is a homogeneous eigenvalue equation which contrasts with an inhomogeneous integral equation for the open lattice. This difference comes from the fact that there exists only scattering state for the open lattice, while there is only bound state for the periodic lattice. Let us define the $N$th-order polynomial $F(x)$ such that

$$\begin{aligned} F(x) &= \mathrm{i}^{-N} D(\mathrm{i}x) \\ &= \prod_{i=1}^{N}(x-\varepsilon_i) = \sum_{k=0}^{[N/2]} A_{2k}x^{N-2k} . \end{aligned} \tag{20}$$

Taking the logarithm of (20), dividing by $N$ and taking the large-$N$ limit, one can get

$$\int_{-Q}^{Q}\ln(x-y)\rho(y)\,\mathrm{d}y = \ln x + \lim_{N\to\infty}\frac{1}{N}\ln(1 + A_2x^{-2} + A_4x^{-4} + \cdots) . \tag{21}$$

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

$$\begin{aligned} -\tfrac{1}{2}\langle\varepsilon^2\rangle &= \lim_{N\to\infty}\frac{1}{N}A_2 \\ -\tfrac{1}{4}\langle\varepsilon^4\rangle &= \lim_{N\to\infty}\frac{1}{N}(A_4 - \tfrac{1}{2}A_2^2) \\ -\tfrac{1}{6}\langle\varepsilon^6\rangle &= \lim_{N\to\infty}\frac{1}{N}(A_6 - A_4A_2 + \tfrac{1}{3}A_2^3) \end{aligned} \tag{22}$$

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

$$A_{2k} \approx a_{2k,k}N^k + a_{2k,k-1}N^{k-1} + \cdots + a_{2k,1}N. \tag{23}$$

Inserting equation (23) into equation (22) and comparing the $N^{l-1}$th $(1\leqslant l\leqslant k)$ order, one can get the following relations for $k\leqslant 3$:

$$\begin{aligned} &a_{2,1} = -\tfrac{1}{2}\langle\varepsilon^2\rangle \\ &a_{4,2} = \tfrac{1}{2}a_{2,1}^2 \qquad a_{4,1} = -\tfrac{1}{4}\langle\varepsilon^4\rangle \\ &a_{6,3} = a_{4,2}a_{2,1} - \tfrac{1}{3}a_{2,1}^3 \qquad a_{6,2} = a_{4,1}a_{2,1} \qquad a_{6,1} = -\tfrac{1}{6}\langle\varepsilon^6\rangle . \end{aligned} \tag{24}$$

Similar equations can be obtained for $k\geqslant 4$ step by step although they become more and more involved. Therefore, once the integral equation (19) is solved and the value $Q$ and the density $\rho(x)$ are given, one can calculate the expectation values $\langle\varepsilon^n\rangle$ and obtain the coefficients $a_{2k,l}$ $(1\leqslant l\leqslant k)$ recursively by (24). Finally the asymptotic expansion of $A_{2k}$ is given by (23).

## 4. Semiclassical quantization

In this section, we will carry out the semiclassical quantization by the EBK (Einstein–Brillouin–Keller) formulation. In this formulation, the quantization conditions are expressed in terms of action variables which are equal to certain areas of the phase space, and it is intuitively very instructive to understand how the zeros of Hill's determinant behave as the number of particles increases.

Since the Toda lattice is integrable, the Hamiltonian can be rewritten in terms of the action-angle variables $(I_i, \theta_i)$ by the canonical transformation. Once the action-angle variables $(I_i, \theta_i)$ are given, the EBK quantization is performed simply by setting $I_i = (n_i + \frac{1}{2})h$. The action variable $I_i$ is expressed by the canonical conjugate variables $(\nu_i, \mu_i)$ [1] as

$$I_i = \oint \nu_i(\mu_i)\, \mathrm{d}\mu_i \,. \tag{25}$$

The auxiliary spectra $\mu_i$ are defined by the eigenvalues of the reduced matrix $L^*$ which is the $(N-1)\times(N-1)$ matrix given by removing the first row and the first column from the matrix $L$ (equation (3)). They are confined in $N-1$ intervals satisfying $|P(\mu)| \geqslant 2$ (they are labelled as $\mu_1 < \mu_2 < \cdots < \mu_{N-1}$). The function $P(\mu)$ is an $N$th-order polynomial with coefficients $A_i$ as $P(\mu) = \sum_i A_i (2\mu)^{N-i}$. The momentum variable $\nu_i$ conjugate to $\mu_i$ is

$$\nu_i = 2(-1)^{N-i} \ln\left|\tfrac{1}{2}\left\{P(\mu_i) + \left[P(\mu_i)^2 - 4\right]^{1/2}\right\}\right| \tag{26}$$

where the positive branch of $[P(\mu_i)^2 - 4]^{1/2}$ is on the upper Riemann sheet. The integral of (25) is carried out in the bounded region where $|P(\mu)| \geqslant 2$. One should note that the function $P(x)$ is related to $D(x)$ (equation (7)) as $P(x) = \mathrm{i}^{-N} D(2\mathrm{i}x)$.

The ground state has quantum numbers $n_1 = n_2 = \cdots = n_{N-1} = 0$ and the quantization conditions are $I_i = \oint \nu_i\, \mathrm{d}\mu_i = h/2 = \pi$ since $\hbar = 1$. These conditions show that each area $\oint \nu_i\, \mathrm{d}\mu_i$ is the same and equal to $\pi$. The practical calculations and the behaviour of $P(\mu)$ will be discussed in the next section.

## 5. Results and discussion

Before getting into the details of the numerical calculation, let us consider qualitative features of the large-$N$ limit of the Hamiltonian. If the exponential potential is truncated by the second order, i.e. $\mathrm{e}^q \simeq 1 + q + \frac{1}{2}q^2$, 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 and eigenfunctions are easily obtained. The ground state energy of the harmonic chain is $E_{\mathrm{hc}}(N) = N + \cot(\pi/2N)$ (The constant energy term $N$ is added in order to compare with the Toda lattice), and thus the $N \to \infty$ limit of the energy per particle is $\lim_{N\to\infty} E_{\mathrm{hc}}(N)/N = 1 + 2/\pi \simeq 1.6366$. If we approximately calculate the ground-state energy of the periodic Toda lattice in the first-order perturbation by employing the ground state eigenfunction $\Phi_{\mathrm{hc}}$ of the harmonic chain, then

$$E_{\mathrm{Toda}}(N) \simeq \langle \Phi_{\mathrm{hc}} | H_{\mathrm{Toda}} | \Phi_{\mathrm{hc}} \rangle = \tfrac{1}{2}\cot(\pi/2N) + N \exp\left(\frac{1}{2N}\cot(\pi/2N)\right) \tag{27}$$

and the energy per particle approaches $\lim_{N\to\infty} \langle \Phi_{\mathrm{hc}} | H_{\mathrm{Toda}} | \Phi_{\mathrm{hc}} \rangle / N = 1/\pi + \exp(1/\pi) \simeq 1.6931$. Therefore the exponential interaction is more repulsive as a whole and the exact value of the energy per particle is expected to be $1.6366 < \lim_{N\to\infty} E_{\mathrm{Toda}}(N)/N < 1.6931$ since higher order perturbations will reduce the expectation value $\langle \Phi_{\mathrm{hc}} | H_{\mathrm{Toda}} | \Phi_{\mathrm{hc}} \rangle$.

Now let us show the numerical results. Equation (19) is a homogeneous Fredholm equation of the second kind. The kernel is $K(x-y) = \Re\psi(1 + \mathrm{i}(x-y))$ and

$$\Re\psi(1 + \mathrm{i}u) = -\gamma_E + u^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2 + u^2)} \qquad (|u| < \infty) \tag{28}$$

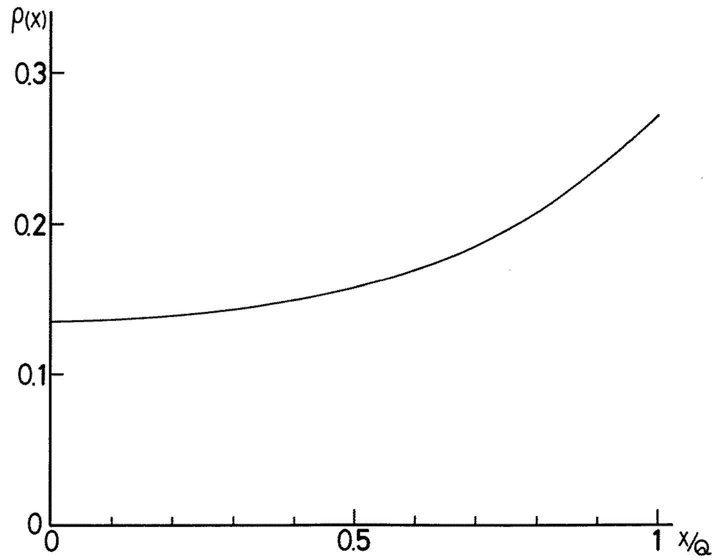


**Figure 1.** Density distribution $\rho(x)$ of the imaginary part of the zeros of Hill's determinant in the large-$N$ limit. $x$ is measured in units of $Q$ $(Q \simeq 2.8992)$ and only the $x \geqslant 0$ region is shown since the function $\rho(x)$ is symmetric.

where $\gamma_E = 0.5772\ldots$ is Euler's constant. Since the kernel is free from singularities, it can be numerically solved easily. Equation (19) is a kind of eigenvalue problem, i.e. one should search for an eigenvalue $Q$ such that there exists an eigenfunction $\rho(x)$. We have done the calculation using two methods, i.e. one is to employ the Gauss–Legendre quadratures and discretize the integral equation, and the other is to expand the kernel in terms of the Legendre polynomials. Both of them are numerically easily performed. The eigenvalue is $Q \simeq 2.8992$ and the eigenfunction $\rho(x)$ is shown in figure 1. The density of the imaginary part of the zeros tends to distribute over the outer region of the interval.

In order to carry out the exact calculation of the spectrum, we must search $[N/2]$ eigenvalues $(A_2 = -E, A_4, A_6, \ldots)$ which satisfy Gutzwiller's quantization conditions simultaneously. We will employ the simplex method with initial values given by the asymptotic expansion. We have calculated the exact eigenvalues up to $N = 20$ and they are compared with the asymptotic expansions of (23) in table 1. Since $A_{2k}$'s diverge as $\mathrm{O}(N^k)$ for $N \to \infty$, we listed the values $A_{2k}/N^k$. For a fixed $k$ the agreement certainly becomes better for larger $N$, while it is better for smaller $k$ when $N$ is fixed. For example, even the sign is opposite for some cases for $2k = N$ when $N \geqslant 12$. Except for the marginal cases (maximum $k$ for a fixed $N$), the agreement is fairly good and one can conclude that the asymptotic expansions are good approximations. The asymptotic value of the energy is $\lim_{N\to\infty} E_{\mathrm{Toda}}(N)/N \simeq 1.6762$, which agrees with our simple estimation mentioned above. The asymptotic values of the conserved quantities are reached very slowly when $k$ becomes large. In figure 2 we show the distributions of the imaginary part of the zeros of Hill's determinant for $2 \leqslant N \leqslant 20$. They tend to distribute over the outer region as $N$ increases and there seems to be an upper bound. One can also see that the $j$th outermost zero moves smoothly as a function of $N$. These exact calculations clearly support the asymptotic behaviour of the zeros of Hill's determinant shown in figure 1.

**Table 1.** Conserved quantities $A_{2k}/N^k$ ($1 \leqslant k \leqslant 10$) for $2 \leqslant N \leqslant 20$. The values in the parentheses are those of asymptotic expansions, while those in the square brackets are semiclassical eigenvalues. $N \to \infty$ asymptotic values are shown at the bottom of the table.

| $N$ | $A_2/N$ | $A_4/N^2$ | $A_6/N^3$ | $A_8/N^4$ | $A_{10}/N^5$ |
|---|---|---|---|---|---|
| 2 | −1.5296 | | | | |
| | (−1.6762) | | | | |
| | [−1.5152] | | | | |
| 3 | −1.6125 | | | | |
| | (−1.6762) | | | | |
| | [−1.5916] | | | | |
| 4 | −1.6406 | 0.2954 | | | |
| | (−1.6762) | (0.2634) | | | |
| | [−1.6164] | [0.2909] | | | |
| 5 | −1.6535 | 0.5000 | | | |
| | (−1.6762) | (0.4917) | | | |
| | [−1.6272] | [0.4900] | | | |
| 6 | −1.6605 | 0.6442 | −0.033 75 | | |
| | (−1.6762) | (0.6439) | (−0.039 60) | | |
| | [−1.6328] | [0.6291] | [−0.033 05] | | |
| 7 | −1.6646 | 0.7500 | −0.078 77 | | |
| | (−1.6762) | (0.7526) | (−0.081 15) | | |
| | [−1.6361] | [0.7305] | [−0.076 69] | | |
| 8 | −1.6674 | 0.8305 | −0.1252 | 0.002 744 | |
| | (−1.6762) | (0.8341) | (−0.1265) | (0.001 948) | |
| | [−1.6381] | [0.8075] | [−0.1213] | [0.002 670] | |
| 9 | −1.6692 | 0.8937 | −0.1692 | 0.008 165 | |
| | (−1.6762) | (0.8975) | (−0.1702) | (0.007 889) | |
| | [−1.6395] | [0.8677] | [−0.1634] | [0.007 898] | |
| 10 | −1.6705 | 0.9444 | −0.2095 | 0.015 50 | −0.000 1731 |
| | (−1.6762) | (0.9482) | (−0.2105) | (0.015 44) | (−0.000 2672) |
| | [−1.6405] | [0.9160] | [−0.2018] | [0.014 93] | [−0.000 1675] |
| 11 | −1.6715 | 0.9862 | −0.2459 | 0.024 04 | −0.000 6267 |
| | (−1.6762) | (0.9897) | (−0.2469) | (0.024 07) | (−0.000 6636) |
| | [−1.6411] | [0.9556] | [−0.2364] | [0.023 05] | [−0.000 6022] |
| 12 | −1.6723 | 1.0211 | −0.2787 | 0.033 20 | −0.001 387 |
| | (−1.6762) | (1.0243) | (−0.2797) | (0.033 28) | (−0.001 405) |
| | [−1.6416] | [0.9886] | [−0.2674] | [0.031 72] | [−0.001 326] |
| 13 | −1.6728 | 1.0506 | −0.3082 | 0.042 59 | −0.002 434 |
| | (−1.6762) | (1.0536) | (−0.3092) | (0.042 71) | (−0.002 446) |
| | [−1.6420] | [1.0166] | [−0.2952] | [0.040 58] | [−0.002 316] |
| 14 | −1.6733 | 1.0759 | −0.3347 | 0.051 97 | −0.003 722 |
| | (−1.6762) | (1.0787) | (−0.3356) | (0.052 11) | (−0.003 734) |
| | [−1.6423] | [1.0405] | [−0.3202] | [0.049 39] | [−0.003 529] |
| 15 | −1.6737 | 1.0979 | −0.3586 | 0.061 16 | −0.005 204 |
| | (−1.6762) | (1.1004) | (−0.3595) | (0.061 32) | (−0.005 218) |
| | [−1.6426] | [1.0613] | [−0.3427] | [0.058 00] | [−0.004 917] |
| 16 | −1.6740 | 1.1171 | −0.3802 | 0.070 06 | −0.006 832 |
| | (−1.6762) | (1.1194) | (−0.3812) | (0.070 23) | (−0.006 848) |
| | [−1.6428] | [1.0795] | [−0.3630] | [0.066 33] | [−0.006 437] |
| 17 | −1.6742 | 1.1341 | −0.3999 | 0.078 62 | −0.008 565 |
| | (−1.6762) | (1.1362) | (−0.4008) | (0.078 80) | (−0.008 584) |

**Table 1.** Continued.

| $N$ | $A_2/N$ | $A_4/N^2$ | $A_6/N^3$ | $A_8/N^4$ | $A_{10}/N^5$ |
|---|---|---|---|---|---|
| | [−1.6429] | [1.0956] | [−0.3815] | [0.074 32] | [−0.008 049] |
| 18 | −1.6744 | 1.1492 | −0.4178 | 0.086 80 | −0.010 37 |
| | (−1.6762) | (1.1511) | (−0.4186) | (0.086 99) | (−0.010 39) |
| | [−1.6431] | [1.1098] | [−0.3983] | [0.081 94] | [−0.009 72] |
| 19 | −1.6746 | 1.1627 | −0.4342 | 0.094 61 | −0.012 21 |
| | (−1.6762) | (1.1645) | (−0.4350) | (0.094 80) | (−0.012 24) |
| | [−1.6431] | [1.1225] | [−0.4136] | [0.089 18] | [−0.011 43] |
| 20 | −1.6748 | 1.1749 | −0.4492 | 0.1020 | −0.014 08 |
| | (−1.6762) | (1.1765) | (−0.4500) | (0.1022) | (−0.014 11) |
| | [−1.6433] | [1.1341] | [−0.4277] | [0.0961] | [−0.013 15] |
| $\infty$ | (−1.6762) | (1.4048) | (−0.7849) | (0.3289) | (−0.1103) |

| $N$ | $A_{12}/N^6$ | $A_{14}/N^7$ | $A_{16}/N^8$ | $A_{18}/N^9$ | $A_{20}/N^{10}$ |
|---|---|---|---|---|---|
| 12 | 0.8938E−5 | | | | |
| | (−0.4926E−6) | | | | |
| | [0.8589E−5] | | | | |
| 13 | 0.3808E−4 | | | | |
| | (0.3451E−4) | | | | |
| | [0.3636E−4] | | | | |
| 14 | 0.9637E−4 | −0.3901E−6 | | | |
| | (0.9509E−4) | (−0.1225E−5) | | | |
| | [0.9150E−4] | [−0.3724E−6] | | | |
| 15 | 0.1890E−3 | −0.1913E−5 | | | |
| | (0.1888E−3) | (−0.2240E−5) | | | |
| | [0.1786E−3] | [−0.1814E−5] | | | |
| 16 | 0.3178E−3 | −0.5449E−5 | 0.1475E−7 | | |
| | (0.3182E−3) | (−0.555 88−5) | (−0.5091E−7) | | |
| | [0.2990E−3] | [−0.5139E−5] | [0.1399E−7] | | |
| 17 | 0.4820E−3 | −0.1182E−4 | 0.8181E−7 | | |
| | (0.4829E−3) | (−0.1190E−4) | (0.5621E−7) | | |
| | [0.4519E−3] | [−0.1110E−4] | [0.7709E−7] | | |
| 18 | 0.6792E−3 | −0.2170E−4 | 0.2591E−6 | −0.4921E−9 | |
| | (0.6806E−3) | (−0.2177E−4) | (0.2491E−6) | (−0.5148E−8) | |
| | [0.6347E−3] | [−0.2028E−4] | [0.2428E−6] | [−0.4637E−9] | |
| 19 | 0.9062E−3 | −0.3555E−4 | 0.6168E−6 | −0.3045E−8 | |
| | (0.9080E−3) | (−0.3562E−4) | (0.6134E−6) | (−0.4880E−8) | |
| | [0.8441E−3] | [−0.3306E−4] | [0.5746E−6] | [−0.2850E−8] | |
| 20 | 0.1159E−2 | −0.5360E−4 | 0.1228E−5 | −0.1062E−7 | 0.1468E−10 |
| | (0.1161E−2) | (−0.5370E−4) | (0.1228E−5) | (−0.1137E−7) | (−0.2855E−9) |
| | [0.1077E−2] | [−0.4970E−4] | [0.1139E−5] | [−0.9881E−8] | [0.1375E−10] |
| $\infty$ | (0.3080E−1) | (−0.7376E−2) | (0.1545E−2) | (−0.2878E−3) | (0.4824E−4) |

In the calculation of the semiclassical quantization, $[N/2]$ semiclassical eigenvalues have been found also by the simplex method and they turn out very close to the exact values. Numerical values are also shown in table 1 in order to compare with the exact values and the asymptotic expansions. In figure 3, we show the characteristic polynomial $P(\mu)$. Since $P(\mu)$ varies very rapidly, we plot the modified discriminant $m(\mu)$ introduced

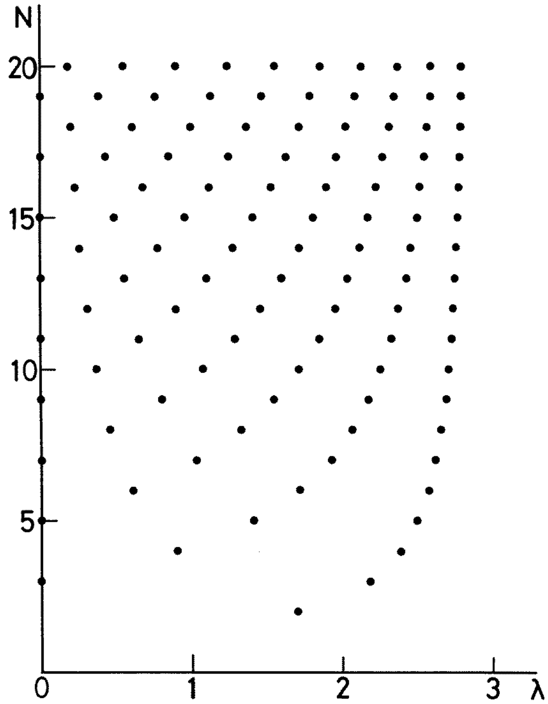


**Figure 2.** Distributions of the imaginary part of the zeros of Hill's determinant for $2 \leqslant N \leqslant 20$. Only non-negative zeros are shown since the distribution is symmetric.

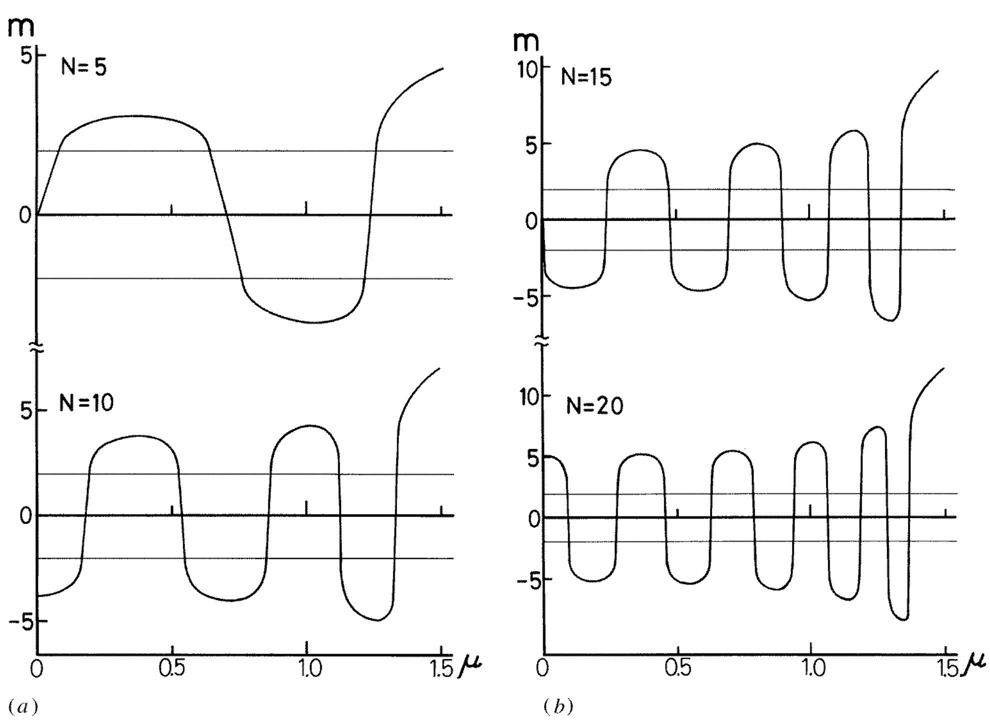


**Figure 3.** Modified discriminant $m(\mu)$ for $N = 5$, 10, 15 and 20. Since $m(\mu)$ is an even (odd) function for $N =$ even (odd), only the $\mu \geqslant 0$ region is shown. Thin lines indicate $|m(\mu)| = 2$.

by Ferguson *et al* [18], which is defined by

$$m(\mu) = \begin{cases} P(\mu) & |P(\mu)| \leqslant 2 \\ \operatorname{sign}(P(\mu)) \left\{ 2 + \frac{2}{\pi} \ln \frac{1}{2} \left( |P(\mu)| + \left[ P(\mu)^2 - 4 \right]^{1/2} \right) \right\} & |P(\mu)| \geqslant 2\ . \end{cases} \tag{29}$$

In this definition, the area $|P(\mu)| \geqslant 2$ is equal to $\frac{1}{2}$ and one can clearly see that the zeros of $|P(\mu)|$ accumulate in the outer region.

## 6. Summary

Based on Gutzwiller's formulation of the quantum periodic Toda lattice, we have derived an integral equation for the density distribution of the zeros of Hill's determinant in the large-$N$ limit. This equation is similar to the Bethe ansatz equation for the open Toda lattice in a box in the thermodynamic limit. However, the integral equation is of inhomogeneous type for the open lattice, while it is a homogeneous eigenvalue equation for the periodic lattice. Making use of the density distribution function, we have calculated the asymptotic expansions of the conserved quantities. The exact eigenvalues are calculated by the simplex method with initial values given by the asymptotic expansions, which turned out to be fairly good approximations. We have also carried out the semiclassical quantization by the EBK formulation. The semiclassical eigenvalues are also found to be very close to the exact values.

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