CALCULATION OF THE ENERGY SPECTRUM OF THE QUANTUM PERIODIC THREE-PARTICLE TODA LATTICE

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The quantum periodic three-particle Toda lattice is considered. For its Hamiltonian, the energy spectrum is calculated in terms of the orthogonal basis in Cartesian coordinates. The eigenstates are classified according to the irreducible representations of the C_{3v}-point group. The spectral statistical properties are analyzed and shown to demonstrate a fairly good agreement with the theoretical predictions for the integrable system.

1. Introduction

Recent achievements in the theory of classical Hamilton systems induced the increased interest in the investigation of the correlation between the dynamical features of a classical Hamilton system and the spectral properties of its quantum counterpart. It was shown in [1] that the distribution $P(s)$ of spacings s between the nearest-neighbour energy levels of an integrable classical Hamiltonian exhibits the Poisson behaviour: $P(s) = \exp\{-s\}$. While, for non-integrable systems exhibiting the chaotic motion, the spectral properties of its quantum counterpart are well described by the random-matrix theory [2]. In particular, the nearest-neighbour spacing distribution has the form proposed by Wigner: $P(s) = \pi s/2 \exp\left\{-\pi s^2/4\right\}$. However, the above-mentioned correlations between the types of classical motion (regular or chaotic) and spectral statistics are not universal [3].

In the present work, the quantum mechanical periodic three-particle Toda lattice is considered. As known [4], this system is integrable in the classical limit. Its Hamiltonian depends on two variables after the separation of the center of mass. We aim at studying the signatures of integrability in the quantum periodic three-particle Toda lattice by analyzing the statistical properties of its spectrum.

The quantum energy spectrum was calculated by the direct diagonalization in the orthogonal basis in Cartesian coordinates. The eigenstates were classified according to the irreducible representations of the C_{3v}-point group. The nearest-neighbour spacing distribution $P(s)$ and the Dyson's $\Delta_3(L)$-rigidity were calculated for each symmetry class of the three-particle Toda Hamiltonian [5]. We did not use a truncated expansion of the Hamiltonian in calculations of the spectrum, as it was done in [6], though, the calculation with the exact potential function took a large amount of computational time and storage. Isola et al. [7] performed similar calculations, but the full symmetry of the Hamiltonian was not taken into account.

2. Classical Periodic Three-particle Toda Lattice

The Toda lattice is the nonlinear dynamical system of n particles of equal masses, interacting each with its nearest neighbour by the exponential law [4]. The classical Hamiltonian of the periodic (the first and last particles are coupled) three-particle Toda lattice may

be written as follows:

$$H = \frac{1}{2m}\sum_{i=1}^{3} p_{x_i}^2 + V_0\left[\exp\left\{\alpha(x_1 - x_2)\right\} + \right.$$

$$\left. + \exp\left\{\alpha(x_2 - x_3)\right\} + \exp\left\{\alpha(x_3 - x_1)\right\}\right]. \qquad (1)$$

Here, m is the mass of a particle, V_0 is the amplitude, and α is the parameter of interaction. We obtain the new form of Hamiltonian (1) with a diagonal quadratic part via the generating function

$$F_2(x_1, x_2, x_3, p_1, p_2, p_3) = \frac{x_1 - x_3}{\sqrt{2}} p_1 +$$

$$+\sqrt{\frac{2}{3}}\left(\frac{x_1 + x_3}{2} - x_2\right) p_2 + \frac{x_1 + x_2 + x_3}{\sqrt{3}} p_3. \qquad (2)$$

The new canonically conjugate coordinates (q_i, p_i) are connected to the old ones (x_i, p_{x_i}) in a following manner:

$$p_{x_i} = \frac{\partial F_2}{\partial x_i}, \quad q_i = \frac{\partial F_2}{\partial p_i}, \quad (i = 1, 2, 3). \qquad (3)$$

Particularly, from equalities (3) we get

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & -\sqrt{\frac{2}{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}. \qquad (4)$$

The same transformation takes place for the canonically conjugate momenta. Let λ_0, τ_0, and ε_0 be the unit of length, time, and energy, respectively. We choose

$$\lambda_0 = \frac{2}{\sqrt{3}\alpha}, \ \tau_0 = \frac{1}{\alpha}\sqrt{\frac{m}{3V_0}}, \ \varepsilon_0 = 4V_0\ , \qquad (5)$$

where τ_0 is the period of the two-dimensional oscillator, ε_0 is the energy of dissociation of the Toda system (1) truncated to the third order in q_1, q_2. The total momentum $P = p_1 + p_2 + p_3$ of system (1) is a conserved quantity. Setting $q_1 \to y$, $q_2 \to x$, $p_1 \to p_y$, $p_2 \to p_x$, we proceed to the following dimensionless form of the classical Hamiltonian (1):

$$H = \frac{1}{2}\left(p_x^2 + p_y^2\right) + \frac{1}{4}\left(\exp\left\{\sqrt{2}x + \sqrt{\frac{2}{3}}y\right\} + \right.$$

$$\left. + \exp\left\{-\sqrt{2}x + \sqrt{\frac{2}{3}}y\right\} + \exp\left\{-2\sqrt{\frac{2}{3}}y\right\}\right). \qquad (6)$$

Hamiltonian (6) describes the classical integrable system with two degrees of freedom. The first few terms of the Taylor expansion of Hamiltonian (6) are:

$$H - \frac{3}{4} = \frac{1}{2}\left(p_x^2 + p_y^2\right) + \frac{1}{2}\left(x^2 + y^2\right) +$$

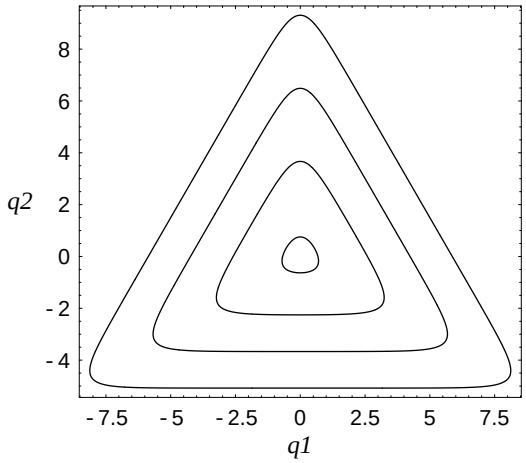

Fig. 1. Contour plot of the potential of the Toda Hamiltonian (6) (contours shown for $E = 1, 10, 100, 1000$)

$$+\frac{1}{\sqrt{6}}\left(x^2 y - \frac{1}{3}y^3\right) + \frac{1}{12}\left(x^2 + y^2\right)^2 + \ldots \qquad (7)$$

Note that the right part of (7) gives the harmonic oscillator in the second order approximation and it gives the Hénon–Heiles term in the third-order approximation.

In 1974, M. Hénon [8] and H. Flaschka [9] found the third integral of motion for the three-particle Toda system. In the case of Hamiltonian (6), it has the form:

$$F = \frac{4}{3}\ p_x\left(p_x^2 - 3p_y^2\right) + \left(p_x - \sqrt{3}p_y\right) \times$$

$$\times \exp\left\{\sqrt{2}x + \sqrt{\frac{2}{3}}y\right\} + \left(p_x + \sqrt{3}p_y\right) \times$$

$$\times \exp\left\{-\sqrt{2}x + \sqrt{\frac{2}{3}}y\right\} - 2p_x \exp\left\{-2\sqrt{\frac{2}{3}}y\right\}. \qquad (8)$$

The contour lines of the Toda potential are shown in Fig. 1. The potential has the symmetry of the C_{3v}-point group which is the symmetry group of an equilateral triangle. The Poincaré cross sections for the three-particle Toda Hamiltonian show that, for any energy E, classical orbits stay on an invariant torus which characterizes the system as being integrable [10]. The cross sections calculated for different energies via the third integral of motion (8) are shown in Fig. 2.

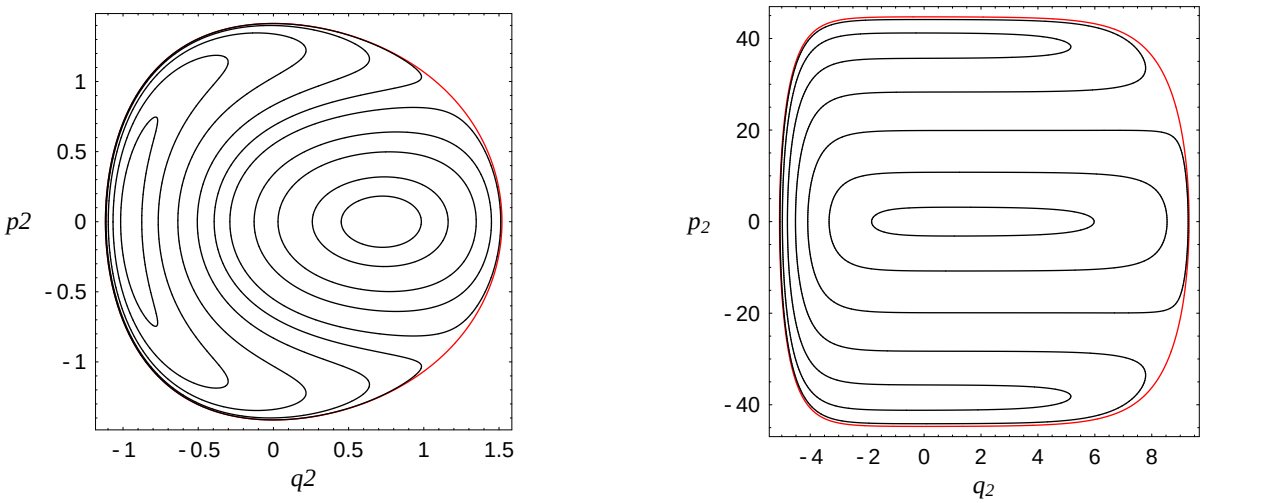

Fig. 2. Cross sections for Hamiltonian (6), calculated via the third integral of motion (8) for energies $E = 1$ (left) and $E = 1000$ (right)

3. Quantum Energy Spectrum Calculation

In the quantum mechanical consideration, the momenta p_x, p_y are replaced by the operators $\hat{p}_x$, $\hat{p}_y$ via the known formulae $p_x \to \hat{p}_x = -i\partial/\partial x$, $p_y \to \hat{p}_y = -i\partial/\partial y$, and the quantum Hamiltonian of the three-particle Toda lattice reads

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{4}\left(\exp\left\{\sqrt{2}x + \sqrt{\frac{2}{3}}y\right\} + \right.$$

$$\left. + \exp\left\{-\sqrt{2}x + \sqrt{\frac{2}{3}}y\right\} + \exp\left\{-2\sqrt{\frac{2}{3}}y\right\}\right). \qquad (9)$$

The units of energy and length in formula (9) are the same as in the classical case, but the additional parameter arises in the quantum case due to the appearance of the Planck's constant. The energy spectrum dependence of this additional parameter was discussed in [6, 7]. In the present work, numerical calculations were performed for Hamiltonian (9).

In order to find the energy spectrum of $\hat{H}$, the eigenvalue problem

$$\hat{H}(x,y)\psi(x,y) = E\psi(x,y) \qquad (10)$$

should be solved. We calculated the energy spectrum by diagonalizing the Hamiltonian matrix $\langle n_1', n_2'|\hat{H}|n_1, n_2\rangle$ in terms of the orthogonal basis $|n_1, n_2\rangle$ in Cartesian coordinates. We did not use truncated expansions of Hamiltonian (9), as it was done in [6].

It is important to take the full symmetry of Hamiltonian (9) into account for two reasons. First, the Hamiltonian matrix $\langle n_1', n_2'|\hat{H}|n_1, n_2\rangle$ can be divided into submatrices corresponding to the different irreducible representations of the symmetry group of Hamiltonian (9) [11]. This allows calculating the eigenvalues for each symmetry type separately. Secondly, it is necessary to distinguish the energy levels belonging to different symmetry types in the analysis of spectral statistical properties [12].

The full symmetry of Hamiltonian (9) is the C_{3v}-point group [11]. It has three irreducible representations: A_1, A_2, and E. The eigenvalues corresponding to A_1 and A_2 symmetries are non-degenerate, while those of E symmetry are doubly degenerate.

We chose the basis functions in Cartesian coordinates as

$$\psi_{n_1 n_2}(x,y) =$$

$$= \frac{1}{\left(\sqrt{2}\right)^{\delta_{n_1 n_2}+1}}\left(u_{n_1 n_2}(x,y) \pm u_{n_2 n_1}(x,y)\right), \qquad (11)$$

where

$$u_{n_1 n_2}(x,y) = \langle x, y|n_1, n_2\rangle =$$

$$= \frac{1}{\left(\sqrt{2}\right)^{n_1+n_2}}\frac{1}{\sqrt{n_1! n_2!}}\sum_{k_1=0}^{n_1}\sum_{k_2=0}^{n_2}(-1)^{n_2-k_2}C_{n_1}^{k_1}C_{n_2}^{k_2}\times$$

$$\times i^{n_1+n_2-k_1-k_2}\sqrt{(k_1+k_2)!}\sqrt{(n_1+n_2-k_1-k_2)!}\times$$

$$\times\phi_{n_1+n_2-k_1-k_2}(x)\phi_{k_1+k_2}(y), \qquad (12)$$

$$\phi_n(t) = \frac{1}{\sqrt{2^n n!}} \sqrt[4]{\frac{\omega}{\pi}} \exp\left\{-\frac{\omega}{2}t^2\right\} H_n(t\sqrt{\omega}), \qquad (13)$$

and $H_n(t)$ is the n-th degree Chebyshev–Hermite polynomial; the sign $+(-)$ in (11) is for $n_1 \geq n_2$ ($n_1 < n_2$), and ω is the fitting parameter. The eigenstates of Hamiltonian (9) are classified according to the irreducible representations of the C_{3v}-point group as shown in the Table below. Note that the quantity L is the angular momentum.

The non-zero matrix elements may be calculated using the orthogonality relation for the functions $\phi_n(x)$ together with the recursion relation for Chebyshev–Hermite polynomials as

$$\left\langle n_1', n_2' \middle| \hat{H} \middle| n_1, n_2 \right\rangle =$$

$$= \frac{1}{\left(\sqrt{2}\right)^{\delta_{n_1 n_2} + \delta_{n_1' n_2'} + 2}} \cdot \frac{1}{\sqrt{2^{N+N'}}} \cdot \frac{1}{\sqrt{n_1! n_2! n_1'! n_2'!}} \times$$

$$\times \sum_{k_1=0}^{n_1} \sum_{k_2=0}^{n_2} \sum_{k_1'=0}^{n_1'} \sum_{k_2'=0}^{n_2'} \left((-1)^{n_2-k_2} \pm (-1)^{n_1-k_1}\right) \times$$

$$\times \left((-1)^{n_2'-k_2'} \pm (-1)^{n_1'-k_1'}\right) C_{n_1}^{k_1} C_{n_2}^{k_2} C_{n_1'}^{k_1'} C_{n_2'}^{k_2'} \times$$

$$\times i^{N-K+N'-K'} \sqrt{(N-K)!(N'-K')!K!K'!} \times$$

$$\times f(N-K, N'-K', K, K'), \qquad (14)$$

$$(N = n_1+n_2, K = k_1+k_2, N' = n_1'+n_2', K' = k_1'+k_2'),$$

where the positive sign in the first (second) parenthesis is taken for $n_1 \geq n_2$, ($n_1' \geq n_2'$) and the negative sign is taken otherwise. The function f in expression (14) is defined as

$$f(m_1, m_1', m_2, m_2') = \omega(m_1+m_2+1)\delta_{m_1 m_1'}\delta_{m_2 m_2'} -$$

$$-\frac{\omega}{4}\delta_{m_2 m_2'} \left\{ \sqrt{(m_1+1)(m_1+2)}\delta_{m_1', m_1+2} + \right.$$

$$\left. +(2m_1+1)\delta_{m_1', m_1} + \sqrt{m_1(m_1-1)}\delta_{m_1', m_1-2} \right\} -$$

$$-\frac{\omega}{4}\delta_{m_1 m_1'} \left\{ \sqrt{(m_2+1)(m_2+2)}\delta_{m_2', m_2+2} + \right.$$

$$\left. +(2m_2+1)\delta_{m_2', m_2} + \sqrt{m_2(m_2-1)}\delta_{m_2', m_2-2} \right\} +$$

$$+\frac{1}{4} \left\{ a_{m_1' m_1}\left(\sqrt{\frac{2}{\omega}}\right) a_{m_2' m_2}\left(\sqrt{\frac{2}{3\omega}}\right) + a_{m_1' m_1}\left(\sqrt{-\frac{2}{\omega}}\right) \times \right.$$

$$\left. \times a_{m_2' m_2}\left(\sqrt{\frac{2}{3\omega}}\right) + \delta_{m_1' m_1} a_{m_2' m_2}\left(-2\sqrt{\frac{2}{3\omega}}\right) \right\}, \qquad (15)$$

where δ is the Kronecker symbol,

$$a_{nm}(y) = \sqrt{2^{m-n}} \sqrt{\frac{n!}{m!}} \frac{y^{n-m} e^{y^2/4}}{(n-m)!} \times$$

$$\times M\left(-m, n-m+1; -\frac{y^2}{2}\right), \qquad n \geq m, \qquad (16)$$

and $M(\alpha, \beta; z)$ is a confluent hypergeometric function [13].

In practical calculations, the elements of the Hamiltonian matrix were ordered by the value of $N = n_1 + n_2$, $N = 0, 1, \ldots, N_{\max}$. We calculated the matrix elements by choosing $N_{\max} = 250$ (for A_1- and A_2-symmetry types) and $N_{\max} = 175$ (for E-symmetry type).

The diagonalization of Hamiltonian (9) was performed via the corresponding procedure of the Mathematica 5.0 package. We obtained 5334 energy levels of A_1-type, 5208 of A_2-type and 5192 of E-type. The accuracy of the results was examined by changing the size of the basis and by varying the fitting parameter ω in (13). We found that $\omega = 2.26$ is optimal and gives about 17% of lowest levels of each type reliable with the accuracy $\delta < 0.1\, s_{\min}$ ($s_{\min}$ is the minimum spacing between nearest-neighbour levels).

The numerical calculations were performed on a Celeron PC and took a large amount of computational time and storage. For example, the diagonalization of the 5192×5192 matrix of E-type took 1781.22 sec. For each type of energy spectrum in terms of the "unfolded" spectrum $\{x_i\}$, the nearest-neighbour spacing distribution $P(s)$ and the Dyson's $\Delta_3(L)$-rigidity were calculated [2]. The histogram $P(s)$ and the $\Delta_3(L)$-rigidity for A_1- and E-symmetry types along with the theoretical curves are shown in Figs. 4, 5.

Classification of the eigenstates according to the irreducible representations of the C_{3v}-point group

Symmetry	$L = n_1 - n_2$
A_1	$L = 0$ or $\begin{cases} L = 0 \pmod 3, \\ L < 0 \end{cases}$
A_2	$\begin{cases} L = 0 \pmod 3, \\ L > 0 \end{cases}$
E	$E_1: \begin{cases} L \neq 0 \pmod 3, \\ L < 0 \end{cases}$ $E_2: \begin{cases} L \neq 0 \pmod 3, \\ L > 0 \end{cases}$

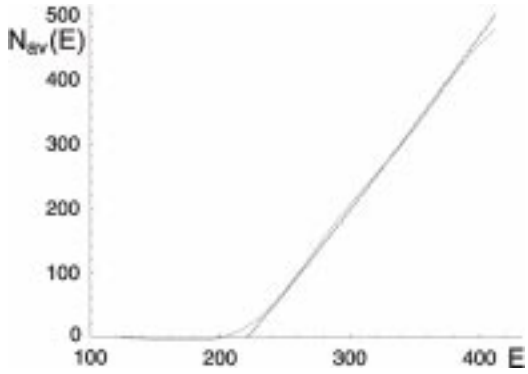

Fig. 3. Staircase function $N(E)$ and function $N_{\rm av}(E)$ calculated for energy levels of the A_1 type (levels from 400 to 900)

4. Spectrum Unfolding and the $\Delta_3(L)$-rigidity

The spectral statistical analysis is applied to spectral fluctuations, i.e. spectrum deviations from its smooth (locally uniform) behaviour [2, 5]. The distribution function (the staircase function) $N(E)$ for a discrete spectrum can be written as

$$N(E) = N_{\rm av}(E) + N_{\rm fluct}(E), \tag{17}$$

where $N_{av}(E)$ is the average part and $N_{fluct}(E)$ is the fluctuation part of $N(E)$. Since the smooth behavior is not universal, it is removed by the spectrum "unfolding" procedure via the mapping [14]

$$x_n + \frac{1}{2} \equiv N_{\rm av}(E_n). \tag{18}$$

We calculated $N_{\rm av}(E)$ in terms of a few lower-order spectral moments by using a truncated Gram—Charlier expansion [15] for the distribution $F(x)$ of the normalized quantity $x = (E - m_E)/\sigma$ (m_E is the expectation, σ is the standard deviation of the spectrum $\{E_i\}$):

$$N_{\rm av}(x) = d \cdot F(x), \tag{19}$$

where d is the total number of levels,

$$F(x) \approx \frac{1}{2}\left(1 + {\rm Er}f\left(x/\sqrt{2}\right)\right) - \frac{\exp\left\{-x^2/2\right\}}{\sqrt{2\pi}} \times$$

$$\times\left(\gamma_a(x^2-1) + \gamma_e x(x^2-3)\right), \quad x = \frac{E - m_E}{\sigma}, \tag{20}$$

γ_a is the skewness, γ_e is the kurtosis excess, ${\rm Er}f(t)$ is the error function [15]. Fig. 3 illustrates $N_{\rm av}(E)$ calculated for the energy levels of A_1-type. In terms of the unfolded spectrum $\{x_i\}$, the spacings between the nearest-neighbour levels are calculated as $s_i \equiv x_{i+1} - x_i$.

The Dyson's $\Delta_3(L)$-statistics measures the spectral rigidity (i.e. the least-squares deviation of the staircase function $N(E)$ from the best fitting line) and is defined [2] on the interval $[\alpha, \alpha + L]$ by

$$\Delta_3(\alpha; L) \equiv \min_{A,B} \frac{1}{L} \int_{\alpha}^{\alpha+L} \left[N(x) - (Ax + B)\right]^2 dx. \tag{21}$$

We use the following formula for numerical calculations [2]:

$$\Delta_3(\alpha; L) = \frac{n^2}{16} - \frac{1}{L^2}\left[\sum_{i=1}^{n} \tilde{x}_i\right]^2 + \frac{3n}{2L^2}\left[\sum_{i=1}^{n} \tilde{x}_i^2\right] -$$

$$-\frac{3}{L^4}\left[\sum_{i=1}^{n} \tilde{x}_i^2\right]^2 + \frac{1}{L}\left[\sum_{i=1}^{n} (n - 2i + 1)\tilde{x}_i\right]. \tag{22}$$

Here, $\tilde{x}_i = x_i - (\alpha + L/2)$ are the shifted unfolded eigenvalues, and n is the number of levels in the interval $[\alpha, \alpha + L]$.

The $\Delta_3(L)$-rigidity is calculated then as

$$\Delta_3(L) = \frac{1}{N_\alpha} \sum_i \Delta_3(\alpha_i; L), \tag{23}$$

where α_i are chosen in such a way that the interval $[a, b]$ containing the unfolded eigenvalues $\{\tilde{x}_i\}$ is split into non-overlapping intervals of length L, $(L \le b - a)$, and N_α is the total number of intervals.

The Dyson's $\Delta_3(L)$-rigidity for integrable systems with the Poisson quantum spectrum is close to $\Delta_3(L) \sim L/15$, while it is $\Delta_3(L) \sim (1/\pi^2)\ln L - 0.00695$ for systems with a quantum spectrum well described by the random-matrix theory, namely by statistical properties of the Gaussian orthogonal ensemble (GOE) [14].

5. Results and Conclusions

In the present work, the quantum periodic three-particle Toda lattice was considered. It was found that the energy spectrum of this system maintains the universal properties of a generic integrable system. Namely, the spacing distribution $P(s)$ of nearest-neighbour levels for each symmetry type is close to the Poisson distribution $P(s) = \exp\{-s\}$ and the $\Delta_3(L)$-rigidity is close to the $\Delta_3(L) \sim L/15$ for $0 \le L \le L_{\rm max}$. The value $L_{\rm max}$ is explained in [16] as the point, at which the $\Delta_3(L)$-statistics saturates (i.e. flattens out at a finite L). We did not calculate the value of $L_{\rm max}$ in the present work, though it can be estimated from Figs. 4 and 5 to be $L_{\rm max} \sim 6$ for the A_1 type and $L_{\rm max} \sim 8$ for the E type.

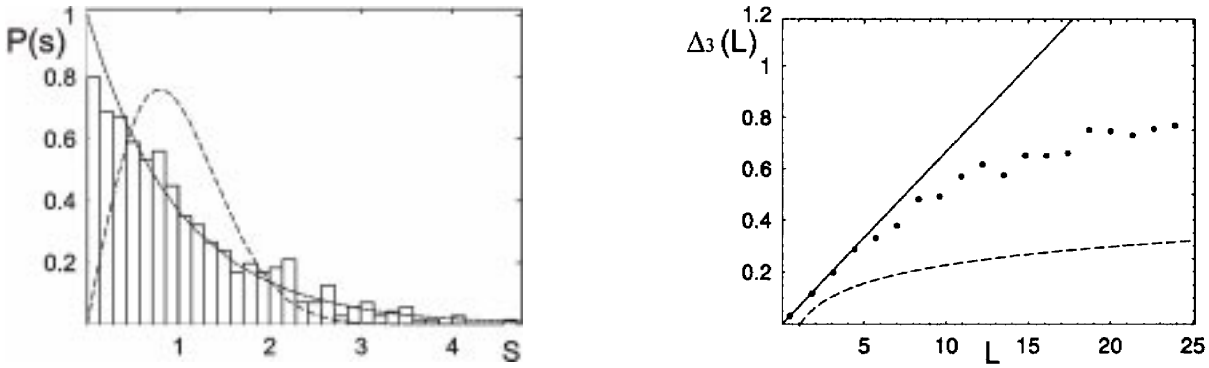

Fig. 4. Nearest-neighbour spacing distribution $P(s)$ and the spectral rigidity $\Delta_3(L)$ for the levels of A_1-type. The total number of levels is 501 (from level 400 to 900). The number of bins in the histogram is 32. The solid line is the Poisson distribution $P(s) = \exp\{-s\}$ in the left graph and $\Delta_3(L) = L/15$ in the right graph. The dashed line is the Wigner distribution $P(s) = \pi s/2 \exp\{-\pi s^2/4\}$ in the left graph and $\Delta_3(L) = (1/\pi^2)\ln L - 0.00695$ in the right graph

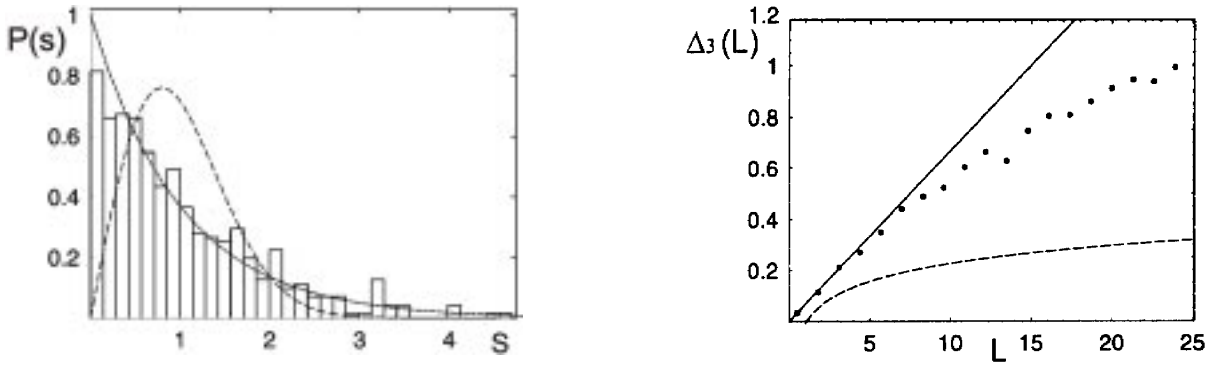

Fig. 5. Nearest-neighbour spacing distribution $P(s)$ and the spectral rigidity $\Delta_3(L)$ for levels of the E-symmetry type. The total number of levels is 501 (from level 500 to 1000). The number of bins in the histogram is 32. The theoretical lines are the same as in Fig. 4

These estimated values for $L_{\max}$ can be explained by the fact that the energy levels included for the spectral statistical analysis are taken from a relatively low part of the Toda spectrum and, thus, may still demonstrate some harmonic behaviour.

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ОБЧИСЛЕННЯ ЕНЕРГЕТИЧНОГО СПЕКТРА КВАНТОВОГО ПЕРІОДИЧНОГО ТРИЧАСТИНКОВОГО ЛАНЦЮЖКА ТОДИ

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Р е з ю м е

Розглянуто квантовий періодичний тричастинковий ланцюжок Тоди. Для його гамільтоніана розраховано енергетичний спектр в ортогональному базисі двовимірного осцилятора в декартовій системі координат. Власні значення класифіковані згідно з незвідними зображеннями точкової C_{3v}-групи. Проаналізовано спектральні статистичні властивості та доведено, що вони достатньо добре узгоджуються з теоретичними передбаченнями для систем, що інтегруються.