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On the quantization of the three-particle Toda lattice

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Received 1 January 1991, in final form 25 March 1991

Abstract. We compare the Einstein–Brillouin–Keller quantization procedure and the canonical quantization of a three-particle Toda chain with periodic boundary conditions. In particular, the transition from very low energies, at which the system may be approximated by harmonic oscillators, to intermediate energies is investigated. This is the regime of a general integrable nonlinear system, for which we find a Poissonian statistics for the energy levels. In the limit of very high energies we exploit the fact that the system may be described essentially by a triangular billiard and thus can derive some exact results.

1. Introduction

The increasing interest in theoretical and experimental aspects of *quantum chaology* marks a revival of old quantum theory. It has been mainly induced by more recent achievements in the theory of classical Hamiltonian systems, where ordered and chaotic motions as well as integrability and ergodicity have become essential ingredients of a coherent theoretical framework. It is natural to wonder what the implications of this complex scenario might be on the quantum properties of these systems. This is the basic question of quantum chaology (Berry 1987). It can be answered by establishing some general correspondence between the spectral properties of a quantum Hamiltonian operator and the dynamical features of its classical limit (Bellissard 1985). One of the main contributions in this direction is due to Berry and Tabor (1977); they have shown that the spectrum of the quantum version of an integrable classical Hamiltonian is characterized by a near-degenerate structure, leading to Poissonian statistics for the level spacing fluctuations. Apart from exceptions like harmonic oscillators (Bleher 1990), this is conjectured to be a generic property of any classically integrable system. Recently, Sinai (1990) has proved this statistical properties for the quantum spectrum corresponding to a geodesic flow on a two-dimensional surface of rotation; moreover he has shown that such properties can be correctly reproduced by the semiclassical approximation. This result provides a relevant contribution in the direction of constructing the quantum analogue of the KAM theorem.

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In contrast, near-degeneracy appears to be highly suppressed in the quantum spectra of ergodic Hamiltonian operators. Numerical analysis on low-dimensional models (Berry 1981, Bohigas *et al* 1984a, b, McDonald and Kaufmann 1979, Casati *et al* 1980) suggests a close analogy between these dynamical systems and random matrices, where eigenvalues statistics is typically Wigner–Dyson like (cf Mehta).

Due to the theoretical and numerical difficulties in studying these problems in full generality, the attention of theoretists has been attracted by simple models. For instance, in two-dimensional billiards it has been possible to obtain a deeper understanding about the relation between the change in level statistics and the transition from ordered to chaotic motion. In particular, the application of semiclassical quantization methods to integrable two-dimensional billiards has provided further insight about the origin of the near-degeneracy mechanism.

Similar investigations have been extended to other low-dimensional nonlinear Hamiltonian models, which exhibit a transition to chaos in their parameter space (e.g. see Pullen and Edmonds 1981, Wintgen and Friedrich 1987). In this respect, classical Hamiltonian chains of nonlinearly coupled oscillators are also good candidates for exploring in detail some general aspects of quantum chaology. At variance with billiards, in the small energy limit these models represent slightly perturbed harmonic chains; consequently, their quantum spectrum near the ground state is expected to show the peculiar degenerate structure of the harmonic case. The first interesting point that we want to discuss in this paper is how such a structure modifies to a near-degenerate one in the highly excited component of the spectrum of an integrable chain. In such a case one can apply also a semiclassical quantization procedure, which is expected to improve as energy increases. In any case, it might be questionable whether this approximate method can reproduce the correct statistics of the spectrum. In the spirit of the Sinai paper (1990), we also discuss this point comparing the results obtained by the *Einstein–Brillouin–Keller (EBK) procedure with the predictions of the canonical quantization*. The object of our investigation is the three-particle Toda lattice. It is the simplest non-trivial version of the prototype of nonlinear integrable chains, the N -particle equal mass Toda lattice. This model was originally introduced in order to study analytic solutions of the equations of motion of nonlinear oscillator systems (Toda 1967). Its integrability was proved some years ago (Hénon 1974, Flaschka 1974) while the analysis of its dynamical properties in terms of action-angle variables has been widely investigated successively (Flaschka and McLaughlin 1976, Ferguson *et al* 1982). In any case, no transformation has been found to separate the Hamilton–Jacobi equation or the associated Schrödinger equation. Nevertheless, wavefunctions of this system have been rigorously studied (Gutzwiller 1980, 1981) by exploiting its symmetry properties.

This paper is organized as follows. In section 2 we briefly report about the integrability of the three-particle Toda lattice. The application of the EBK semiclassical quantization procedure is described in section 3, where we also comment about the validity of this approximate method. Section 4 is devoted to the canonical quantization of the reduced Toda Hamiltonian using the basis of the eigenfunctions of two harmonic oscillators with equal frequencies. In section 5 we compare the results obtained by the two methods, which show a very good agreement over the whole energy scale. Level statistics is discussed in section 6, where we present some exact results obtained in the high energy limit through a geometrical analogy of the three-particle Toda lattice with an equilateral triangular billiard. Conclusions and perspectives are contained in section 7.

2. The classical system

We shall consider a three-particle Toda lattice, described by the Hamiltonian

$$H = \sum_{i=1}^3 \frac{p_i^2}{2} + \exp(q_{i+1} - q_i) - 3 \quad (2.1)$$

with periodic boundary conditions $q_{i+3} = q_i$. This system has three independent conserved quantities, namely total momentum P , energy E and a third invariant

$$I_3 = -p_1 p_2 p_3 + p_1 \exp(q_3 - q_2) + p_2 \exp(q_1 - q_3) + p_3 \exp(q_2 - q_1).$$

It is straightforward to show that they are in involution, so that the system is completely integrable (cf Arnold 1978). Because of translational invariance the two non-trivial action variables J_1, J_2 depend on E and I_3 only. Thus for any value of E, P and I_3 the phase space can be decomposed into the direct product of a two-dimensional torus and a one-dimensional straight line corresponding to the constant growth of the centre of mass variable. In any case an explicit expression of the generating function of the canonical transformation to action-angle variables is unknown. Nevertheless, one can set up a numerical procedure in order to compute the actions corresponding to any value of E and I_3 . To this end, let us recall some known facts. First, the Jacobi matrix L , given by

$$L = \begin{pmatrix} b_1 & a_1 & a_3 \\ a_1 & b_2 & a_2 \\ a_3 & a_2 & b_3 \end{pmatrix} \quad (2.2)$$

where $a_i = \frac{1}{2} \exp((q_{i+1} - q_i)/2)$ and $b_i = \frac{1}{2} p_i$ together with the skew symmetric matrix B

$$B = \begin{pmatrix} 0 & a_1 & -a_3 \\ -a_1 & 0 & a_2 \\ a_3 & -a_2 & 0 \end{pmatrix} \quad (2.3)$$

satisfy the equation

$$\dot{L} = [L, B] \quad (2.4)$$

i.e. L and B form a Lax pair (Arnold 1988, Lax 1968). Therefore the eigenvalues of L as well as the coefficients of the characteristic polynomial are constants of the motion (the latter are related to the invariants explicitly). The characteristic polynomial reads

$$Q(\lambda) = -\lambda^3 + \frac{1}{2} P \lambda^2 + \left(\frac{1}{4}(E+3) - \frac{1}{2} P^2\right) \lambda + \frac{1}{8} I_3 + 2a_1 a_2 a_3.$$

Let us label by $\Lambda_i, i = 1, \dots, 6$, the consecutive intersections of the third-order polynomial

$$\Delta(\lambda) = -8Q(\lambda) + 2 \quad (2.5)$$

with the two horizontal lines passing through ± 2 (see figure 1). Then, one can compute the actions J_1 and J_2 as the integrals (Ferguson *et al* 1982)

$$J_i = \frac{2}{\pi} \int_{\Lambda_{2i}}^{\Lambda_{2i+1}} \cosh^{-1} \left(\frac{|\Delta(\lambda)|}{2} \right) d\lambda. \quad (2.6)$$

Let us notice that the three intersections of $\Delta(\lambda)$ with the upper line are given by the eigenvalues of L , whereas those with the lower line are the eigenvalues of L^- , which is obtained from L by changing the sign of the two elements in the upper right and lower left corners (van Moerbeke 1976).

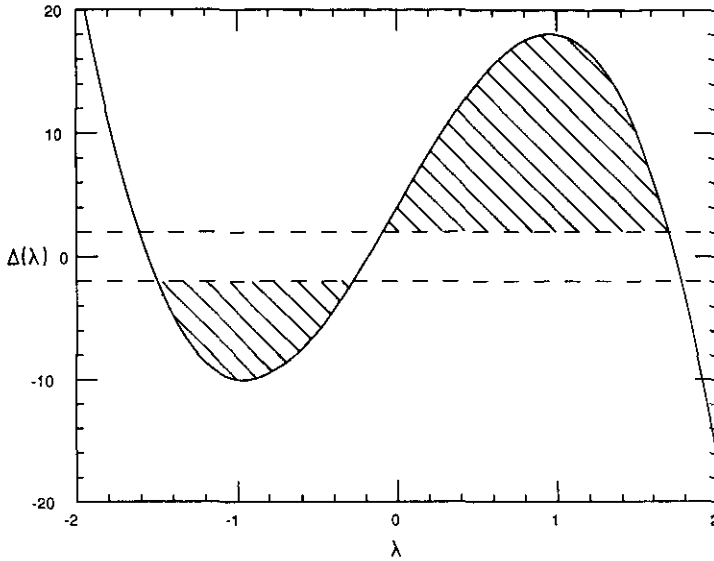


Figure 1. The discriminant $\Delta(\lambda)$ (equation (2.5)) for typical values of the invariants. The area of the shaded regions is in one-to-one correspondence with the actions defined in (2.6).

Thus, although not being algebraic expressions of the phase space coordinates, the actions can be computed numerically for each point in phase space.

3. Semiclassical quantization

As the classical actions are known, one can use the EBK quantization procedure to obtain the semiclassical levels of the system. According to this procedure, a quantal energy state labelled by quantum numbers (m, n) is associated with a torus where J_1 and J_2 assume the values $(m + \alpha_m/4)\hbar$ and $(n + \alpha_n/4)\hbar$, respectively (in the present case, since in the limit of vanishing energy the system reduces to a couple of harmonic oscillators, the Maslov indices α_n and α_m are both equal to 2). In principle, the energy E_{mn} of such a state can be found in terms of the Hamiltonian written as a function of the actions

$$E_{mn} = H(J_1 = (m + \frac{1}{2})\hbar, J_2 = (n + \frac{1}{2})\hbar). \quad (3.1)$$

This semiclassical quantization procedure is known to be valid in the limit $\hbar \rightarrow 0$. More generally, the condition is $E/\hbar \approx l \rightarrow \infty$, where l is the quantum number. For fixed E this corresponds to highly excited states. However, very often it gives accurate results even for the ground state; in particular there are few cases (harmonic oscillators, Coulomb potential, rectangular boxes) where it gives all levels exactly. So, *a priori*, in our case we have two exact limits: near the ground state, where the chain behaves as if it were harmonic, and at very high energies, where the system is composed by three free particles with hard core interaction. In the intermediate region one has to be careful, as the deviation from the harmonic potential increases with the energy, which is a monotonic function of $l\hbar$. Thus, one has to choose \hbar small enough to guarantee that the levels with small quantum numbers have small enough energies to be close to the harmonic case.

In the specific case of the three-particle Toda lattice, as we have seen previously, J_1 and J_2 depend implicitly on the energy and on I_3 . So we can exploit the procedure summarized in (3.1) only numerically by changing the values of E and I_3 in a controlled way, then calculating the corresponding actions and finally retaining those values of E for which J_1 and J_2 satisfy the quantization rule. Algorithmically this is equivalent to looking for zeros in a parameter plane, with the advantage that for each pair (m, n) there exists only one solution. For the sake of simplicity, but without loss of generality, we choose $P = 0$, so that the quadratic term in $Q(\lambda)$ vanishes.

By using a Newton algorithm, with this procedure we have computed the first 6000 levels for $\hbar = 1$, the first 16 000 levels for $\hbar = 0.1$, and the first 2500 levels with $\hbar = 0.01$, with an absolute accuracy of 2×10^{-5} .

4. Canonical quantization

Although the exact quantization conditions for the three-particle Toda lattice have been established (Gutzwiller 1980, 1981), no explicit expression for the spectrum is actually available. Anyway, an exact quantization procedure by which, in principle, one can straightforwardly obtain as many eigenvalues as one wishes (even though, when implemented on a computer, it is only approximate) is the following.

Consider the Hamiltonian operator \hat{H} , obtained from the classical Hamiltonian H by canonical quantization, and compute all transition elements of \hat{H} in a suitable Hilbert space basis. Then, by diagonalizing the resulting (infinite) matrix one finds, in principle, all the eigenvalues of \hat{H} .

Operationally, we first reduce the classical system to two degrees of freedom by separating the motion of the centre of mass, so that the new Hamiltonian reads (see also Ford *et al* 1973)

$$H(u, v, p_u, p_v)$$

$$= \frac{p_u^2}{2} + \frac{p_v^2}{2} + \exp(\sqrt{2}v) + \exp(-\sqrt{\frac{1}{2}}v + \sqrt{\frac{3}{2}}u) + \exp(-\sqrt{\frac{1}{2}}v - \sqrt{\frac{3}{2}}u) - 3. \quad (4.1)$$

The Taylor series expansion of the potential is

$$V(u, v) = \frac{3}{2}(u^2 + v^2) + \frac{1}{2\sqrt{2}}(v^3 - 3u^2v) + \frac{3}{16}(u^4 + 2u^2v^2 + v^4) + \text{HOT}. \quad (4.2)$$

A natural basis for the quantum Hamiltonian is the direct product of two harmonic basis $\{\phi(u)\} \times \{\phi(v)\}$ (with the same frequency $\omega = \sqrt{3}$). Indeed, this choice guarantees the self-adjointness of the operator \hat{H} . Moreover, in the limit of vanishing energy, i.e. when the quadratic part of (4.2) is dominant, the true Toda eigenfunctions are very close to the harmonic ones.

By the way, the first two terms of (4.2) form the Hénon–Heiles system up to rescaling of coordinates and time.

We order the basis elements $\phi_m(u)\phi_n(v)$ according to the total harmonic energy $l = m + n$. More precisely, within a group of $l + 1$ degenerate levels of harmonic energy $(l + 1)\hbar\omega$ we choose an ordering in such a way that the states of our basis are given by

$$\psi_k(u, v) = \phi_m(u)\phi_n(v) \quad \text{with } k = m + 1 + \sum_{l=0}^{m+n} l. \quad (4.3)$$

Of course this is somewhat arbitrary, as a reordering of levels (inside a group) corresponds to an exchange of rows and columns of the matrix $H_{ij} = \langle \psi_i | \hat{H} | \psi_j \rangle$, which does not affect the eigenvalues of H_{ij} . The matrix H_{ij} is symmetric, as \hat{H} is Hermitian.

The computation of the transition elements is straightforward, and gives

$$\langle \phi_m(\xi) | e^{\alpha \hat{\xi}} | \phi_n(\xi) \rangle = \sqrt{\frac{n! m!}{2^n 2^m}} \sum_{l=0}^n \frac{2^l \alpha^{n+m-2l}}{l!(n-l)!(m-l)!} e^{\alpha^2/4} \quad (4.4)$$

where $\hat{\xi} = (\sqrt{\omega/\hbar}) \hat{x}$. A numerical difficulty arises from the occurrence of factorials of large integers. For $\hbar\omega < 2$ transition elements decrease with increasing difference of the quantum numbers in each subspace. Thus, the main entries of the matrix H_{ij} are close to the diagonal. This merely reflects the fact that the most important contributions to the potential come from the first terms of its Taylor expansion (4.2), as each power is suppressed by a factor $\sqrt{\hbar/\omega}$.

Now, since H is invariant under the transformation $u \rightarrow -u$, it conserves the parity of wavefunctions in the u -subspace. Therefore, all transition elements between wavefunctions with different parity in u -space are zero. This allows us to reorder the elements H_{ij} into two blocks of given parity in the u -subspace, which can be diagonalized separately. The corresponding subsets of the basis have m even and m odd, respectively. Moreover, the complete spectrum of H_{ij} consists of many pairs of degenerate eigenvalues and only few non-degenerate ones: the even parity subset gives the whole spectrum without degeneracy, whereas the odd parity subset yields the fellows missing to form the degenerate pairs.

This decomposition into blocks of given parity is still valid for any truncation \bar{H}_{ij} of the infinite matrix. Thus we consider a subset of N basis vectors ψ_k , $k = 1, \dots, N$, where $N = (L+1)(L+2)/2$ is chosen in such a way that all basis elements corresponding to harmonic energies $E_k \leq E_L = (L+1)\hbar\omega$ are included. According to what we have said before, all levels are obtained (apart from degeneracy) by diagonalizing only the submatrix acting on subspace $\{\psi_k, 0 \leq k \leq N, m \text{ even}\}$, which has rank $N_e = \frac{1}{4}L^2 + L + 1$. The number of non-degenerate levels then is $[L/2] + 1$.

By diagonalization of such a finite \bar{H}_{ij} with a routine of the NAG library, we find N_e eigenvalues. The crucial question is, how many of them are good approximations of the eigenvalues of the infinite matrix. From the variational principle it follows (Zimmermann *et al* 1984), that all eigenvalues are upper bounds of the true ones†. The comparison of the eigenvalues computed for different sizes N of the matrix provides an estimate of the number N_e of reliable eigenvalues‡, which depends significantly on N and \hbar (see figure 2). Up to this number, curves for different N coincide with high precision, and, what is more, the mean deviations are much smaller than the average level spacings. Thus the global growth of the energy $E(i)$ as a function of the level number i shows approximately a square root behaviour (exactly as in the semiclassical case) up to $i = N_e$, above which it increases quickly, in the limit $i \rightarrow N$ faster than exponentially.

† For the ground state this can be seen directly. Let $\bar{\psi}_0$ be the ground state of the truncated Hamiltonian \bar{H} . Then

$$\bar{E}_0 = \langle \bar{\psi}_0 | \bar{H} | \bar{\psi}_0 \rangle = \langle \sum \alpha_i \psi_i | \hat{H} - \hat{H}_{\text{res}} | \sum \alpha_i \psi_i \rangle = \sum \alpha_i^2 E_i > E_0$$

as $\langle \bar{\psi}_0 | \hat{H}_{\text{res}} | \bar{\psi}_0 \rangle = 0$, and where ψ_i are the wavefunctions of the complete Hamiltonian and E_i its eigenvalues.

‡ Using a Cray we have computed up to 4560 eigenvalues in 9 minutes. The limitation is given by central memory occupation rather than CPU time.

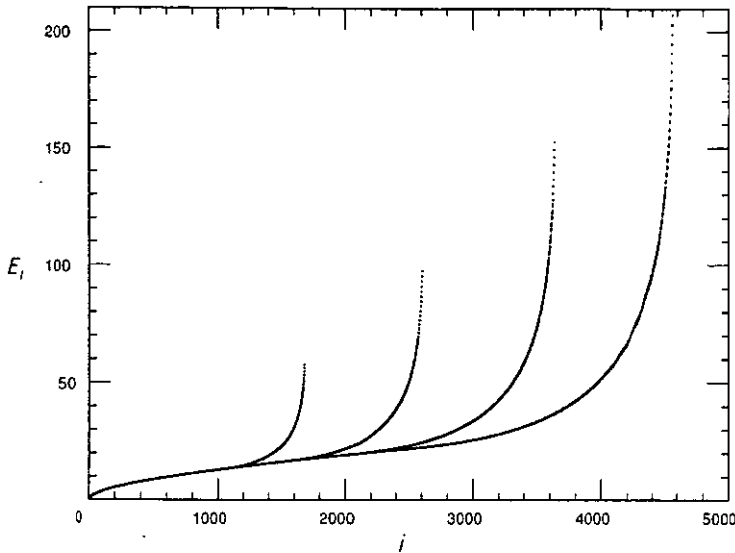


Figure 2. The eigenvalues E_i of the truncated matrix \tilde{H}_i against i , for matrix sizes $N_e = 1681, 2601, 3630, 4775$, with $\hbar = 0.1$.

5. Comparison of the two quantization procedures

There are two semiclassical quantum numbers m, n . From (2.6) and (3.1) it follows that the energy is invariant under the exchange of n and m , whereas I_3 changes its sign. This amounts to shift the graph of $\Delta(\lambda)$ in the vertical direction (see figure 1), so that the upper and lower areas are reversed. Therefore all levels E_{mn} with $m \neq n$ are pairwise degenerate. This means that for any fixed l out of the set of $l+1$ levels with $n+m=l$, exactly one level is non-degenerate if l is even, whereas all levels are twofold degenerate, if l is odd.

Apart from this, there is no other symmetry, which may lead to exact degeneracies, in our semiclassical procedure.

In the canonical quantization procedure we have no knowledge about the quantum numbers of the system: levels are only ordered according to their magnitude. Nevertheless the structure of degeneracies, which we described in section 4, turns out to be exactly the same as the semiclassical one.

Therefore we are allowed to compare the two methods more efficiently ignoring degeneracy. After ordering also the semiclassical levels E_i^s by their magnitude, we have computed the relative deviation from the canonical eigenvalues E_i^c with the same level number

$$\delta_i = (E_i^c - E_i^s) / \sqrt{E_i^c E_i^s}. \quad (5.1)$$

The results for $\hbar = 0.1$ are presented in figure 3, together with the absolute deviations. For the three values of \hbar considered in section 2 we find the same behaviour: the semiclassical levels are always smaller than those obtained by the canonical procedure. For the first levels of the spectrum the deviations δ_i shrink very rapidly with i , up to a given value from which on the decrease is linear with very small slope. In the latter region, the relative deviation is $\mathcal{O}(10^{-4}\hbar)$, whereas the absolute one is $\mathcal{O}(10^{-2}\hbar^2)$. This good agreement ranges up to a level number $i = N_a$, which depends only on the size

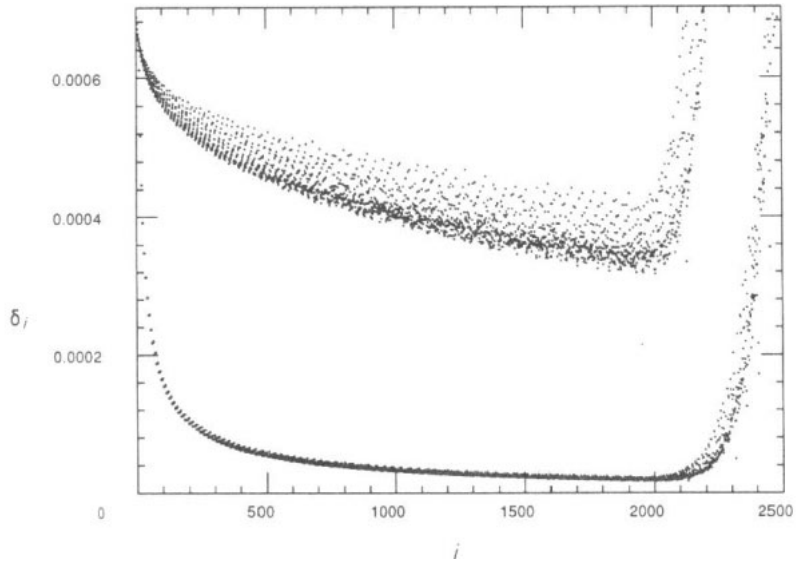


Figure 3. The absolute (upper) and relative (lower curve) deviations δ_i of the semiclassical levels with respect to the canonical ones as a function of the level number i , computed for $\hbar = 0.1$ and $N_e = 4557$.

of the matrix used for the diagonalization procedure and is related to N_a , defined in section 3. Beyond N_a one observes an exponential increase of the deviations with a rate $\mathcal{O}(10^{-3})$. This is simply an effect of the truncation in the canonical procedure and has nothing to do with the reliability of the semiclassical eigenvalues.

As finally we are interested in the level statistics, we also investigated the agreement of the level spacings $\Delta E_i = E_{i+1} - E_i$, i.e. we computed $\Delta_i = (\Delta E_i^s - \Delta E_i^c) / \sqrt{\Delta E_i^s \Delta E_i^c}$.

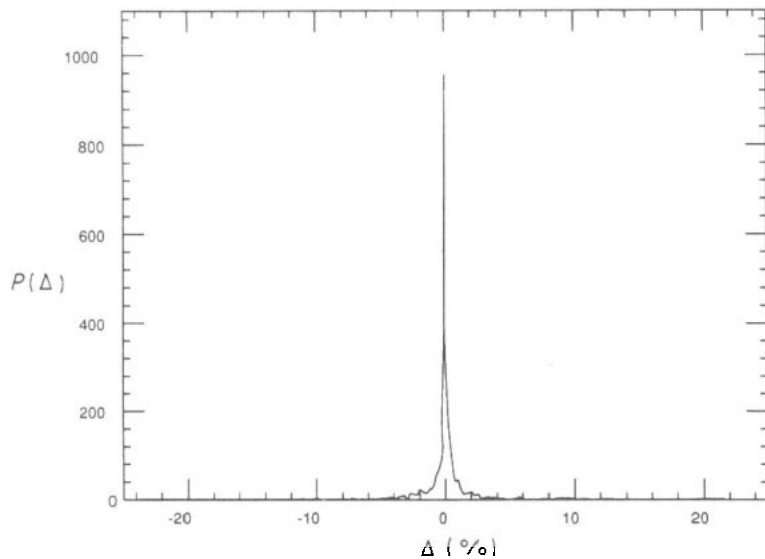


Figure 4. The distribution of the deviations Δ_i of the level spacings obtained with the two methods. The parameters are the same as in figure 3.

The level spacings ΔE_i agree up to less than 1% for most i , single exceptions having some percent deviation. The latter reflects the fact that the semiclassical levels were computed individually with an intrinsic error originating from both the precision of the numerical evaluation of the integrals and the finite precision of the Newton procedure. In figure 4 we have decided to show the distribution of Δ_i values. Indeed, this is more significant than simply showing Δ_i against i .

6. The statistics of levels

Let us consider again the semiclassical quantization procedure, according to which the energies of the quantal states can be found from (2.1). A given state, labelled by quantum numbers (n_0, m_0) , arises from the intersection of the curve $E = H(J_1, J_2)$, considered in the two-dimensional space of quantum numbers (m, n) , with the lattice point (m_0, n_0) . It is just this crossing process that produces the increasing ordered sequence of semiclassical levels

$$0 \leq E_1 \leq E_2 \leq \dots \leq E \leq \dots \quad (6.1)$$

Then, in order to understand the structure of the spectrum (e.g. level spacings, degeneracies etc), it is crucial to know the shape of such a curve as the energy E is varied (see Berry and Tabor 1977). In our case this problem can be solved in the two limits $E \rightarrow 0$ and $E \rightarrow \infty$. Making reference to (4.2), we know that in the first limit the two non-trivial degrees of freedom behave as harmonic oscillators with frequencies $\omega_1 = \omega_2 = \omega = \sqrt{3}$. Consequently, in this limit the levels are well described by

$$E_{m,n} = \hbar\omega(m+n+1) \quad (6.2)$$

i.e. they occur at energies $E = \hbar\omega(l+1)$, $l=0, 1, 2, \dots$ with degeneracies $l+1$. These groups of $l+1$ degenerate levels are separated by gaps of order \hbar , so that the mean spacing between levels, irrespective of the degeneracies, is of order \hbar^2/E . Let us note that, with respect to this mean spacing, the levels arrive at ever-increasing intervals in ever more degenerate groups. However this description is valid only in the limit $E \rightarrow 0$. As soon as the energy is slightly increased the above degeneracies are broken and the spacings between the levels belonging to a given group increase linearly, according to general perturbation theory arguments. This can also be understood by the fact that the contours of constant energy in the plane of quantum numbers get a non-zero curvature as energy increases, and the crossing process is consequently modified. A qualitative idea of the rate at which the curvature moves away from zero can be obtained from figure 5, showing some contours of constant E (for $0 \leq E \leq 66$) in the (m, n) plane, obtained numerically by projecting several intersections of the two-dimensional energy surface with horizontal planes onto the space of (positive) quantum numbers. In this direction, one can also understand qualitatively the mechanism of level crossing, which can always be observed in the spectrum of an integrable system when a given parameter is varied (harmonic oscillators provide an exception in this respect).

Let us start from an energy value where the system is very close to be harmonic, so that the corresponding contour in the (m, n) plane is nearly a straight line (see figure 5). Introducing a control parameter which changes smoothly the strength of the potential or, equivalently, on varying \hbar continuously, the energy contour will smoothly change its curvature (in our case the orientation is preserved by symmetry) so that the

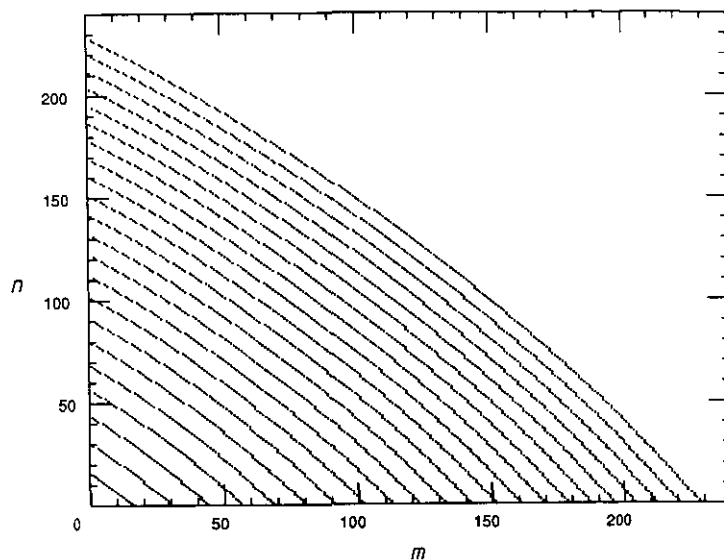


Figure 5. Contours of constant energy, for $0 < E < 66$, in the space of the semiclassical quantum numbers m and n .

lattice points on a $m + n = \text{const}$ line are crossed sequentially as energy increases. Thereafter, there will typically be a value of \hbar where the contour cuts two lattice points located on two successive $m + n = \text{const}$ lines, giving rise to a crossing between levels belonging to different harmonic groups. This behaviour is clearly exhibited in figure 6. Notice that in the diagonalization procedure described in section 3, one cannot see whether two levels have actually crossed, as they are automatically ordered by their amplitude. However, from the semiclassical quantization we can compute the corresponding quantum numbers and thus identify a level crossing unambiguously.

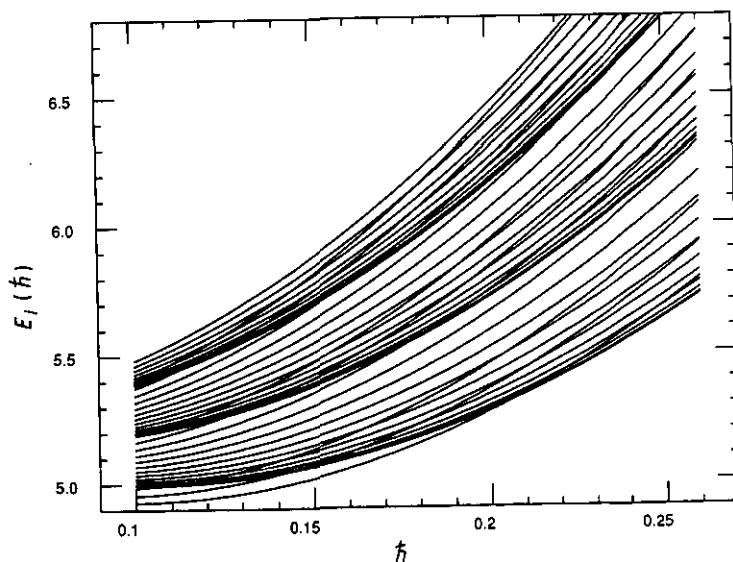


Figure 6. The energies of 40 successive levels as a function of \hbar .

Now, introducing the function $N(E)$, equal to the number of levels E_i which are less than E , one naturally expects that, as E increases, the mechanism of overlap between independent groups of levels will progressively change the behaviour of $N(E)$: from the quasi-harmonic situation, where $N(E)$ is well described by the regular staircase

$$N(E) = \sum_{l=0}^{[E/\hbar\omega]} (l+1) = \frac{([E/\hbar\omega]+1)([E/\hbar\omega]+2)}{2} \quad (6.3)$$

to the highly nonlinear regime, where $N(E)$ behaves as a random function (Berry and Tabor 1977). In order to describe this randomness it is convenient to study the clustering distribution $P_r(k)$ (see Sinai 1990), namely the probability that choosing E at random, the interval $(E, E+r)$ contains k levels. Another, more customary, indicator is the spacing distribution $P(s)$, defined in such a way that $P(s) ds$ gives the probability that the spacing of a randomly chosen pair of neighbouring levels will be between s and $s+ds$, where s is measured as a fraction of the mean spacing at the energy considered.

In our case, we expect that when the energy is sufficiently high, i.e., far above the harmonic region in the spectrum, the clustering distribution is Poissonian,

$$P_r(k) = e^{-r} \frac{r^k}{k!} \quad (6.4)$$

and the spacing distribution is exponential,

$$P(s) = e^{-s}. \quad (6.5)$$

In figures 7 and 8 one can observe a strong numerical evidence of this behaviour. These statistical features of the spectrum appear to be universal for the (non-generic) class of those systems for which the EBK quantization procedure is applicable (Berry and Tabor 1977), even though the precise mechanism underlying this behaviour remains to be clarified in a unified way. However, since the harmonic system provides an

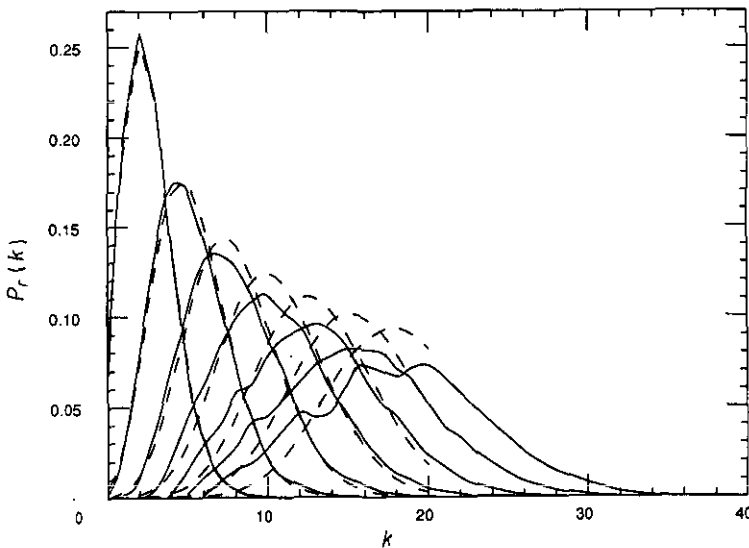


Figure 7. The clustering distribution functions $P_r(k)$ for $r=0.1, 0.2, 0.3, \dots, 0.7$, and $\hbar=0.1$. It has been computed from the first 15 000 semiclassical levels, after discarding the lowest 1000.

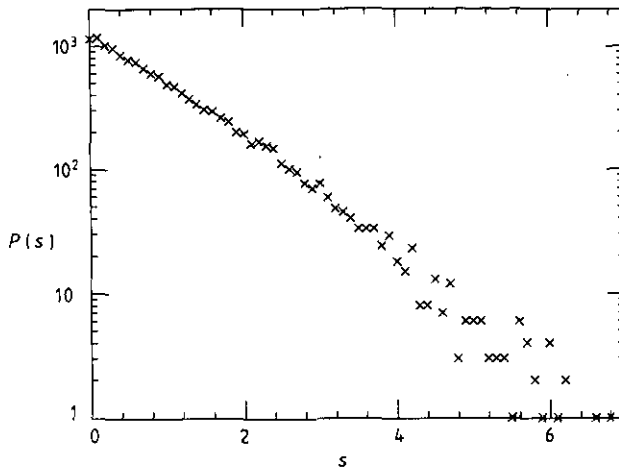


Figure 8. The level spacing distribution $P(s)$, computed with the same data of figure 7.

exception in this respect, also the first part of the Toda spectrum, which represents a slight perturbation of (6.2), does not show the Poissonian behaviour. The latter sets in only when different groups of levels with $m + n = \text{constant}$ overlap strongly. As a matter of fact, figures 7 and 8 represent only this region.

We can partially understand the mechanism leading to the strong clustering property exhibited in figure 7, showing in particular that in the limit of very high energies, this can be related to the degeneracy structure of the sequence of levels (6.1). To this end, let us consider the contour plot of the potential (3.1); see figure 9. For small values of u and v , the equipotential contours are nearly circular, as expected. For larger values of $V(u, v)$, the deviation from the harmonic oscillator potential is significant and, in the limit $E \rightarrow \infty$, the contour describes an equilateral triangle.

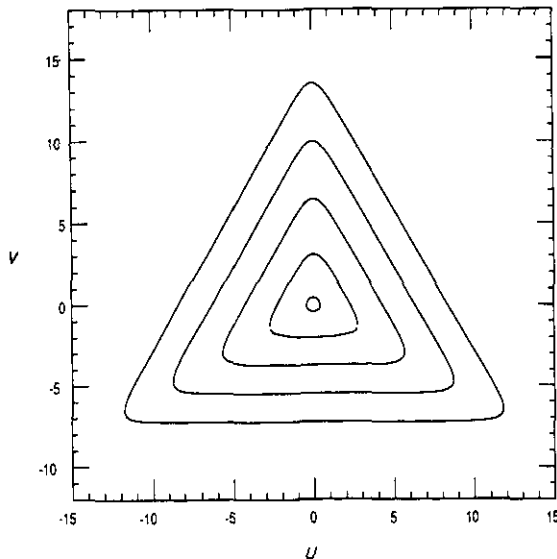


Figure 9. The equipotential lines of the Toda potential (4.1).

Then, as for $E \rightarrow 0$ we have discussed our system in terms of two slightly perturbed harmonic oscillators, in the opposite limit, $E \rightarrow \infty$, we can consider it as essentially equivalent to a particle moving in a two-dimensional triangular billiard.

The eigenvalues of an equilateral triangle of unit side have been obtained in by Lamé (1852) and Pinsky (1980), and for the Dirichlet problem they are given by

$$\lambda_{m,n} = \frac{16\pi^2}{9} (m^2 + n^2 + mn). \tag{6.6}$$

On the other hand, the asymptotic length of the sides of the triangles in figure 9 is

$$L(E) \rightarrow \sqrt{6} \log E \quad \text{as } E \rightarrow \infty. \tag{6.7}$$

This means that in this limit the eigenvalues of our system occur at energies given by

$$E(\log E)^2 = \frac{8\pi^2 \hbar^2}{27} (m^2 + n^2 + mn) \tag{6.8}$$

that is, the asymptotic shape of the energy contours in the (m, n) plane is that of a portion of an ellipse, as shown schematically in figure 10. In polar coordinates this curve takes the form

$$r = \left(1 + \frac{\sin 2\alpha}{2}\right)^{-1/2} k\sqrt{E} \log E \tag{6.9}$$

where $0 \leq \alpha \leq \pi/2$ and $k = (3/2)^{3/2} (1/\pi\hbar)$. The two axes of the ellipse have size

$$a = \frac{3}{\pi\hbar} \sqrt{\frac{3E}{2}} \log E \quad \text{and} \quad b = \frac{a}{\sqrt{3}} \tag{6.10}$$

respectively.

It is worth mentioning that if one interprets (6.8) as a semiclassical formula—like (2.1)—it provides an implicit relation between the energy and the action variables in the classical problem.

Now, in the semiclassical approximation, the function $N(E)$ can be decomposed as

$$N(E) = \bar{N}(E) + N_{\text{osc}}(E) \tag{6.11}$$

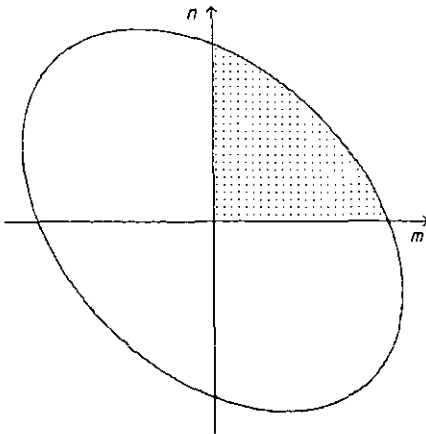


Figure 10. The asymptotic shape of the energy contour in the (m, n) -plane.

where the average term $\bar{N}(E)$ is a smooth function of E and $N_{\text{osc}}(E)$ is a series of oscillatory corrections (Berry 1981). In our case, the first term is given by the number of lattice points contained in the intersection of the ellipse with the first quadrant (see figure 10). On the other hand it is easy to see that the area of this region is

$$\mathcal{A} = \frac{ab}{4} \left(8 \tan^{-1} \left(\frac{a}{b} \right) - \pi \right) \quad (6.12)$$

and thereby we obtain

$$\bar{N}(E) = \frac{15\sqrt{3}}{8\pi\hbar^2} (\log E)^2 E \quad (6.13)$$

which is nothing but the Weyl formula, for $\bar{N}(E)/E$ is proportional to the area of the triangle. We stress however that this result is strictly valid only as $E \rightarrow \infty$.

From (6.13) we have that the mean number of levels contained in $(E, E+r)$ is proportional to $r \log E (2 + \log E) / \hbar^2$, so that the mean spacing between levels shrinks as $\hbar^2 / (\log E)^2$ as $E \rightarrow \infty$. The fact that the mean spacing is not simply a constant $\mathcal{O}(\hbar^2)$, as it is in any two-dimensional bound system, is a consequence of the unbounded size of the triangular billiard we are considering.

Finally, a result obtained by Pinsky (1980) states that if one introduces the functions

$$\begin{aligned} n_k(E) &= \#\{i \mid E_i \leq E: E_i \text{ is } k\text{-fold degenerate}\} \\ n(E) &= \sum_1^\infty \frac{n_k(E)}{k} \end{aligned} \quad (6.14)$$

then for the modes of the equilateral triangle we have

$$\frac{N(E)}{n(E)} \sim \text{constant} \times \frac{E}{\alpha(E)} \quad E \rightarrow \infty \quad (6.15)$$

i.e. the eigenvalues tend to have infinite degeneracy as $E \rightarrow \infty$. This means that, for a triangle of constant size, where the mean spacing is constant, the levels are increasingly degenerate and separated by increasingly large gaps. A similar picture occurs for the rectangular billiard (Berry 1981). For comparison, let us note that for the harmonic system one finds $n(E) = [E/\hbar\omega]$ so that

$$\frac{N(E)}{n(E)} \sim \frac{[E/\hbar\omega]}{2} \quad E \rightarrow \infty \quad (6.16)$$

that is, the degeneracy increases linearly with E .

We argue that, at very high energies, where $(\log E)/E \sim 0$, the levels of the three-particle Toda system follow closely the behaviour expressed by (6.15), which then provides the asymptotic mechanism responsible for the statistical properties observed in figures 7 and 8. A more refined analysis of this mechanism, which would lead to a closer understanding of the underlying random process, implies the knowledge or, at least, a rigorous estimate of the function $N_{\text{osc}}(E)$.

7. Conclusions and perspectives

In this paper we have studied the quantum analogue of the completely integrable three-particle Toda lattice. The comparison between canonical and semiclassical quantization has shown that the latter procedure provides an effective approximation scheme

in reproducing the statistical properties of the spectrum. This is in agreement with the results obtained by Sinai (1990) for the case of integrable two-dimensional geodesic flows. The observed equivalence between the two quantization schemes has allowed us to investigate the level clustering properties in terms of the crossing process of the energy contour in the plane of quantum numbers. We have discussed in detail the small and high energy limits where the system resembles an harmonic chain and an equilateral triangular billiard, respectively. In particular we have obtained strong evidence that far above the ground state the clustering distribution of levels obeys a Poissonian statistics. Such results hold true for different choices of \hbar , which is a free parameter in our model.

A more systematic investigation on the dependence of such results when \hbar is varied together with the analysis of nonlinear oscillator chains with more than three particles will be the subject of further studies. In particular we shall investigate these points also for non-integrable systems; in this perspective it will be interesting to consider the Fermi-Pasta-Ulam α and β models (Fermi *et al* 1965).

Acknowledgments

This work started at the Institute for Scientific Interchange (ISI) in Torino during the workshop 'Chaos and Complexity 1990'. We are indebted to ISI for kind hospitality in a very stimulating research environment. Moreover we wish to thank J Bellissard for discussions and illuminating suggestions. One of us (HK) also wants to acknowledge interesting discussions with B Eckhardt and J Keymer, and the financial support by the Commission of the European Community, DG XII.

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