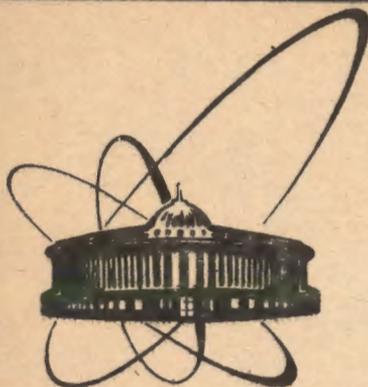


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QUANTUM SPECTRA
OF NON-INTEGRABLE CLASSICAL SYSTEMS
IN TRANSITION TO CHAOS REGION

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1 Introduction

An almost universal property of the deterministic nonlinear dynamics systems is its stochastic behavior pertinent to its nonintegrability. In fact, the chaotic solutions have been well established for an enormous number of evolution equations appearing in all branches of science (e.g. ⁽¹⁾⁻⁽³⁾). The Hamiltonian dynamics takes a prominent role among dynamical systems due to the importance of complete integrability of hamiltonian systems. The N-dimensional Hamiltonian system is completely integrable if there exists N integrals of motion that are in involution with respect to some Poisson bracket structure the classical trajectories winding on N-dimensional torus in the phase space. According to the classical Kolmogorov-Arnold-Moser (KAM) theorem ⁽⁴⁾ the phase space structure is stable under a small non-integrable 'perturbation admixing'.

Discovery of the classical chaotic motion stated the problem of studying quantum manifestations of the classical stochasticity. For a large class of Hamiltonians: two-dimensional model systems, hydrogen atom in a strong external field, etc, the mean dist-

ance between the neighboring spectral values becomes larger and the nearest-neighbor-level spacing distribution evolves from the Poisson to the Wigner distributions, provided that the classical dynamics is passing from the regular to chaotic regime, the total energy being smoothly varying ⁽⁵⁾. Other quantum characteristics, that have not been systematically elaborated but merely used for detecting classical stochasticity, are : statistical properties of eigenfunctions and their nodes, the sensitivity of the spectrum under variation of the nonlinearity strength, the entropy of the level's grouping.

In this paper the quantum spectrum of a two-parameter Hamiltonian flows is studied. In the vicinity of classical energy critical region where the chaos becomes important a reach sets of energy levels quasi-crossings were observed for the quantum Hamiltonian. A characteristic property of these quasi-crossings is that they lay on approximately parabolic curves in parameter space. We investigated the break-up of the spectrum shell structure (with respect to 2dim oscillator quantum numbers) when the strength of the non-integrable perturbation is increasing. In this transition region the violation of quasi-periodic entropy dependence is observed.

Let us examine the behavior of quantum spectrum around the classical energy corresponding to transition from regularity to chaos for a two-dimensional two-parameter Hamiltonian

$$H=1/2(p_x^2+p_y^2)+V(x,y;c,b) \quad (1)$$

where

$$V(x,y;c,b)=\frac{1}{2}(x^2+y^2)+b(x^2y-\frac{1}{3}y^3)+c(x^2+y^2)^2. \quad (2)$$

This Hamiltonian is currently used in hydrodynamical models ⁽⁶⁻⁸⁾ with potentials corresponding to quadruple vibrations of the spherical liquid drop surface. This class of Hamiltonian has the following practical advantages : i) the structure of the classical phase space is well established ⁽⁷⁻⁸⁾; ii) the potential surface is smoothly varying between one-and many



0,8E_{kp}



0,2E_{kp}



1,2E_{kp}

Fig 1. A typical Poincaré sections demonstrating the change of motion for potential (2) the parameter W being in the interval (4,16).

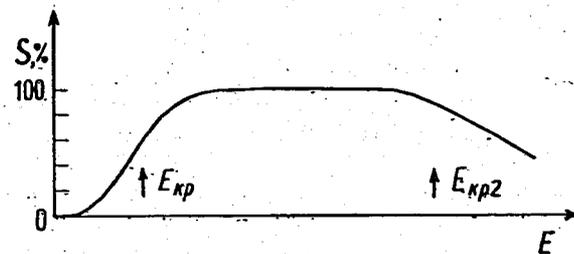


Fig 2. Dependence of the phase space stochastic part (in %) on the energy. The arrows is pointing on the critical energies E_{cr1}, E_{cr2}.

minima potentials when the parameters are continuously varying;
 iii) the classical motion is finite ;
 iv) this class contains both integrable and nonintegrable cases;
 v) owing to the C_{3V} -symmetries the Hamiltonian diagonalization gets much simplified.

The topology of potentials $V(x,y;a,b)$ is governed by the parameter $W=b^2/c$. For b,c in the region $0 < W < 16$ the potential surface reaches an unique minimum at the origin. This corresponds to spherically symmetric equilibrium state. In the region $0 < W < 4$ the Gaussian curvature of the potential surface is positive, the motion being presumably regular and the possible transition to chaos have to be expected only at and beyond the border of this region, where the local instabilities are going to appear together with the negative Gaussian curvature in $4 < W < 16$. The critical energy for transition to chaos in this region agrees with numerical estimates extracted from Poincare sections (see Fig.1)

In Fig.2 the rate of chaotic phase space volume is traced out on the Poincare sections for the Hamiltonian (2) for $W=13$. At low energies the classical system behaves according to the KAM theorem. The phase torus rigidity is dumping the rate of chaotic motion up to critical energy predicted by the negative curvature criterion⁽⁹⁾ for transition to chaos. Energy raising up to value $E \sim E_{cr}$ leads to complete stochasticity, but at $E \sim 10^4 E_{cr}$ the regularity is restored again. Presumably this sort of regularity- chaos- regularity transition is taking place for all systems possessing a locally negative Gaussian curvature⁽⁹⁾, the second critical energy being estimated to a great extent by the upper limit of the negative curvature region. In this paper we concentrate on the character of energy spectrum close to regularity- chaos transition.

When $W \in (0,16)$ the potential surface being one well like, the diagonalization of Hamiltonian (1) can be easily performed in the following orthonormalized bases:

$$|NLj\rangle = 1/\sqrt{2}(|N,L\rangle + j|N,-L\rangle), \quad N=0,2,\dots; \quad L=N,N-2,\dots,1 \text{ or } 0 \quad (3)$$

$$\langle N'L'j' | N L j \rangle = 2^{\delta_{L,0}} \delta_{jj'} \delta_{NN'} \delta_{LL'} \quad (4)$$

Here the functions $|N,L\rangle$ span an orthonormal basis for two-dimensional symmetric oscillator:

$$\langle r, \varphi | N, L \rangle = \frac{i^N e^{-iL\varphi}}{\sqrt{2\pi}} \frac{1}{L!} \sqrt{\frac{2!(N+L)/2!}{(N-L)/2!}} r^L e^{-\frac{r^2}{2}} M\left(-\frac{N+L}{2}, L+1; r^2\right) \quad (5)$$

M being the confluent hypergeometric function⁽¹⁰⁾.

In this basis the matrix elements $\langle N'L'j' | H | N,L,j \rangle$ being invariant under the symmetry group C_{3V} were splitted into direct sum of three blocks labelled by C_{3V} -irreducible representations index. Following the standard notations we will denote the corresponding series of levels by A_1 ($Mod(L,3)=0, j=1, L=0$ included), A_2 ($Mod(L,3)=0, j=-1, L=0$ excluded), E ($Mod(L,3) \neq 0, j=\pm 1$).

The dependence of E-series on parameter of 'nonlinearity' is depicted on Fig 3 for $W=13$. In the case $b=0, c=0$ the well known harmonic oscillator spectrum is observed. The relatively small perturbation $b \neq 0$ is removing the L-degeneracy forming a spectrum shell structure. Moreover N, L remains suitable quantum numbers even though the wave functions cease to be eigenfunctions of \hat{L} and \hat{N} , i.e. the classifications of states remains valid even for large enough nonlinearity b . The numerical results (Fig 3a and Fig.4) obtained for $W=13$ shows that the classification of states remains reasonable in the region where multiple quasicrossings of neighboring levels are taking place¹. The solid curves laying crosswise in Fig 3a,b shows the critical energy bound corresponding to the classical (negative curvature) criterion for transition to chaos. The break-up of the shells becomes important beyond this

¹ Here we call quasi-crossings those points where two energy curves get much closer than the mean level distance.

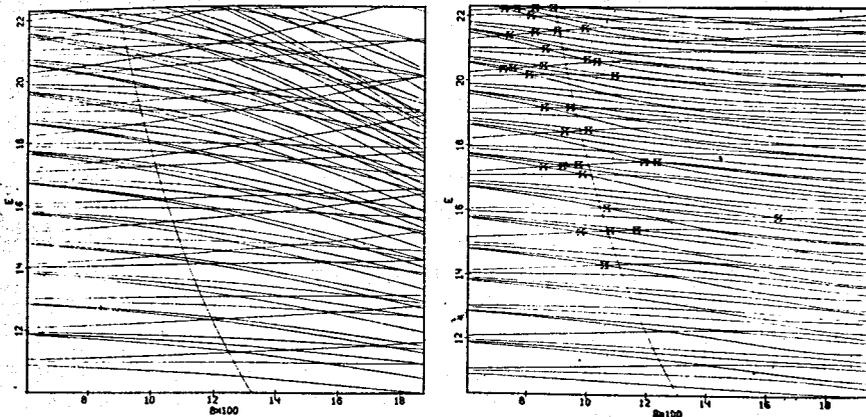


Fig 3. Dependence of energy spectra for (1) on parameter b :
 a) quasi classical spectrum calculated according to formula (6);
 b) the numerical exact spectrum. The squares mark quasi crossings.

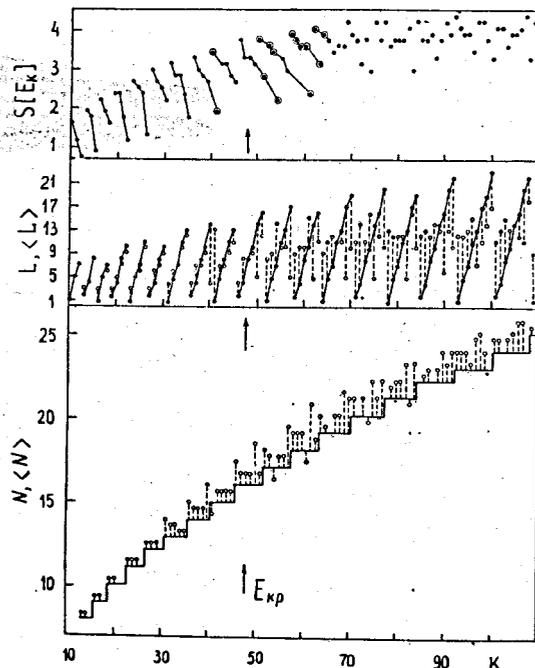


Fig 4. Dependence of the quantities $S, L, \langle L \rangle, N, \langle N \rangle$ on the state number k for $W(4,16)$. Legend $- \circ - \circ S, L; \circ - \circ \langle L \rangle, \langle N \rangle$; correspond to the shell's crossings; the step-wise line is depicting N .

bound. Note that for $W < 4$ the nonlinear perturbation parameter b for which the quasi-crossings were negligible is much larger than that allowed for $W = 13$. This fact can be interpreted as a quantum version of classical KAM theorem⁽¹¹⁾ In Fig 3a is depicted the levels structure computed by the quasiclassical formula of fourth order⁽¹²⁾

$$E(N, L) = N + 1 + b^2 / 12 [7L^2 - 5(N+1)^2 + 1] + c/2 [3(N+1)^2 - L^2 + 1]. \quad (6)$$

The coincidence with the numerical results (Fig 3a) is really remarkable this way strongly arguing that in fourth order approximation to the initial Hamiltonian all quasicrossings are exact crossings at least below the critical energy region. One can trace the destruction of shell structure looking on the entropy of the states⁽¹³⁾, expounding the exact solution in the basis $|N, L, j\rangle$ and introducing the entropy of individual eigenvectors:

$$S[E_k] = - \sum_{N, L, j} |c_{NLj}^{(k)}|^2 \ln |c_{NLj}^{(k)}|^2 \quad (7)$$

the quantities c_{NLj} being determined by expansion over the basis (3)-(5):

$$\langle r, \varphi | E_k \rangle = \sum c_{NLj}^{(k)} \langle r, \varphi | NLj \rangle. \quad (8)$$

The nature of entropy change at energies below the critical transition region to chaos (see Fig 4) is correlated with the transitions from shell to shell. Within individual shell the entropy is monotonically decreasing with increasing of L . As the energy levels get closer to quasicrossing point one observes two phenomena: i) the quasi-periodic dependence of entropy is going to be loosed step-by-step, indicating the shell structure destruction; ii) for energies larger than the critical one, one sees a monotonic growth of the (averaged) entropy ascending to plateau². The smearing of shells can be illustrated by averaging the operators \hat{N}, \hat{L} between unperturbed states (Fig 4) or even better by differences $\Delta N = N - \langle \hat{N} \rangle, \Delta L = \langle \hat{L} \rangle$ depicted in Fig 5. It is clear that at

² This plateau corresponds to purely random sequence.

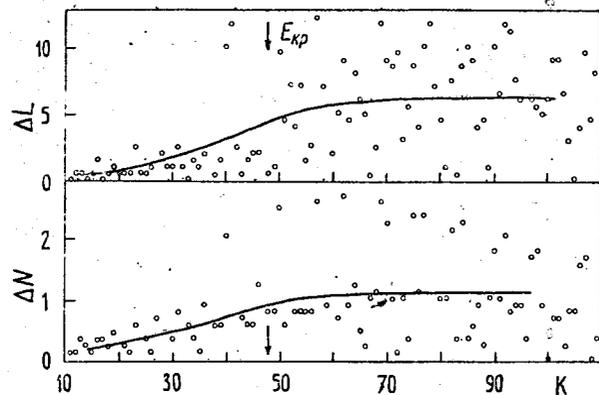


Fig 5. The differences $\Delta N = N - \langle N \rangle$, $\Delta L = L - \langle L \rangle$ as functions on the state number for $W=13$. Legend- $\circ \rightarrow$ values of $\Delta N, \Delta L$; lines \rightarrow the averaged ΔN and ΔL .

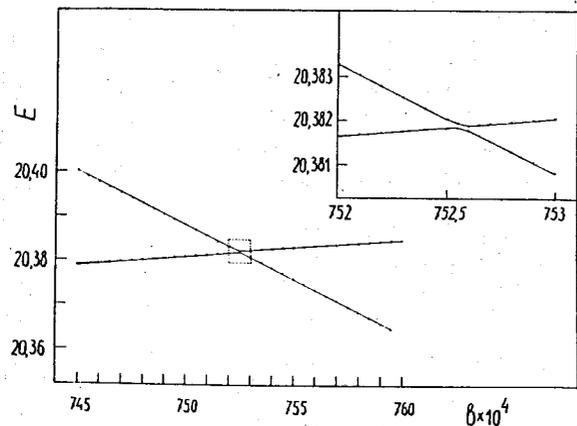


Fig 6. Dependence of ΔE for $k=71$ and 72 on the parameter b , for $c=0,00045$.

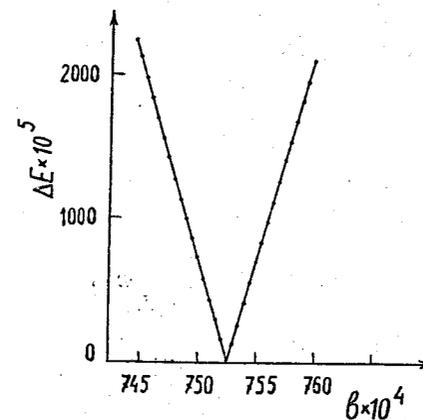


Fig 7. The variation of energy for approaching levels $k=71,72$ with respect to nonlinearity parameter b , c being fixed to $0,00045$.

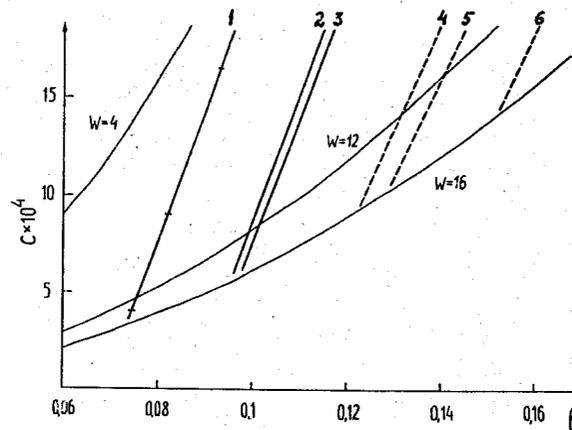


Fig 8. Dependence of some levels quasicrossings on parameters b, c . Here the following legend is used: 1 \rightarrow ($k=71,72$); 2 \rightarrow ($k=40,41$); 3 \rightarrow ($k=60,61$); 4 \rightarrow ($k=34,35$); 5 \rightarrow ($k=39,40$), 6 \rightarrow ($k=47,48$) all computations performed for $E < E_{cr}$, for 1,2,3, whilst 4,5,6 are computed at energy $E > E_{cr}$. The curves tagged by W denote borders between different topologies of the potential (2). By crosses it were marked those values of (b,c) where the wave functions have been computed for purposes of Fig 9.

energies where $\Delta N > 1$ and $\Delta L > 2$ the classifications of levels in terms of quantum numbers L, N become meaningless. This fact is closely related to the level quasicrossings, responsible also for failing of quasiclassical approximation (Eq.(6)).

As an example for quasicrossing we show in Figs.6,7 the b -dependence of the energy levels $E=E_{71}$ and $E=E_{72}$ approaching one another up to 10^{-5} . As the nonlinearity b gets larger, the distance between neighboring energy curves increases which is nothing else but repulsing of levels.

It was observed that the points of minimal distance between nearby curves (1,2,3) lay approximately on parabolae in the plane (b, c) (See Fig. 8). This follows easily by the quasiclassical spectrum (Eq.(6)) the appropriate quantum numbers being replaced in the relation $E_i(b, c) = E_j(b, c)$. The situation becomes more subtle in the stochastic region where N, L lose their proper sense of quantum numbers. Besides that the characteristic "thickness" ΔE of the lines (4,5,6) is of order 10^{-2} which freely speaking can be interpreted as a presence of avoided crossings thereby.

When one passes across some of these lines of minimal distance the wave functions corresponding to the quasicrossing levels are exchanging. This fact is illustrated on the example of levels $k=71$ and $k=72$ close to $b^* = 0,075255$, $c^* = 0,00045$. The modulus squared of the coefficients $C_{NL}^{(k)}$ taken on each side of that line being drawn in Fig 9, demonstrate this exchange.

Note also that the analogous calculations made for A_1, A_2 -levels (See Fig 10,11) demonstrate again reach avoided crossing pictures close to the classical critical energy.

3 The hypothesis for multiply quasicrossings scenario to chaos transition seems plausible also for C_{4V} -symmetric Hamiltonians. The energy spectrum analysis of reduced Yang-Mills Hamiltonian ⁽¹⁴⁾ provides a simple model of this type:

$$H = \frac{1}{2}(p_x^2 + p_y^2) + V(x, y; b, c) \quad (9)$$

$$V(x, y; b, c) = \frac{1}{2}(x^2 + y^2) + bx^2y^2 + c(x^2 + y^2)^2.$$

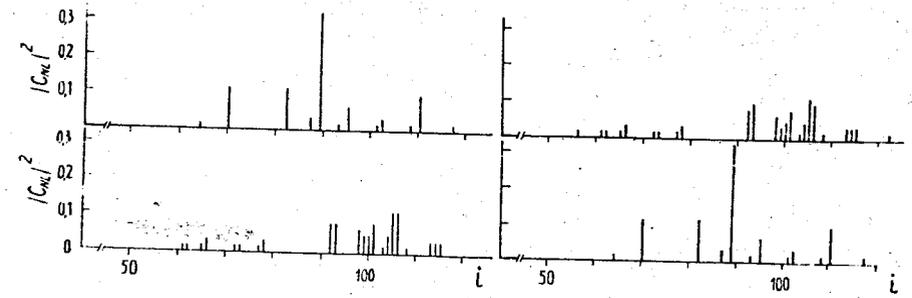


Fig 9. Dependence of coefficients $|C_{NL}^i|^2$ on the number of the basic state i for energy states $k=71, 72$. In the left part $b < b^*$, while the right diagram is obtained for $b > b^*$.

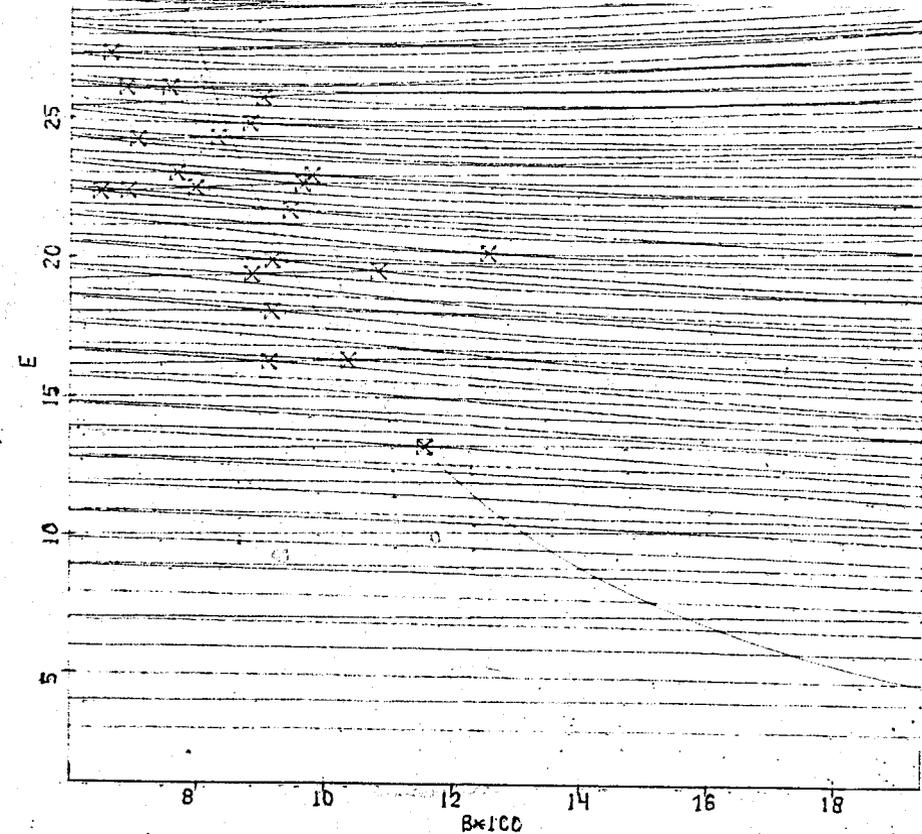


Fig 10. The same as in Fig 3a, but for A_1 spectrum.

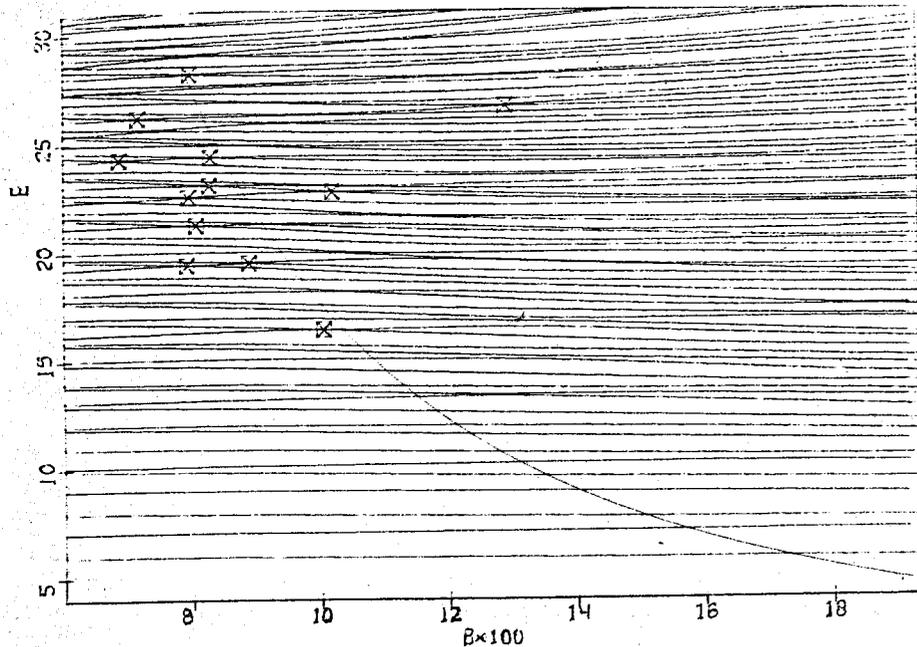


Fig 11. The same as Fig 3a for A_2 spectrum.

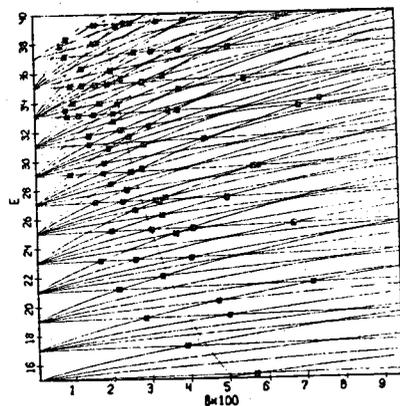


Fig 12. Dependence of exact spectra for the Hamiltonian (9) as function of parameter b . The squares mark quasi-crossings.

The classical energy corresponding to transition to chaos results from the negative Gaussian curvature criterion thereby equals to

$$E_{cr} = \frac{3b-4c}{4(b-4c)^2} \quad (10)$$

For b and c in the interval $4 < b/c < \infty$ and $E > E_{cr}$ the Gaussian curvature vanishes and becomes negative one leading this way to local instabilities and chaotic motion. Fig.12 shows the dependence of A_1 -type levels for $b/c=999$. Obviously here as well as in the C_{3V} -case we have discussed in Sec.2 the quasicrossings are still teeming. Moreover, they also lay along curves. In particular for the levels $k=20,21$ the curve of minimal distances can be quite well interpolated by the line $c=.2055b-.007958$ for $b \in (.003-.004)$.

4. In order to establish whether the observed quasi-crossings are *avoided crossings* or *exact crossing* one should apply to the analytic arguments. It is known that ^(14,15) if there is an accidental degeneracy at some point of the parameter space (called diabolic point) then a circuit walk around should change the sign of the wave function. This rule has been successfully used for identification of diabolic points in the vibration spectrum of a triangular membrane (triangular billiard) ⁽¹⁵⁾. Unfortunately numerical check of this test disproved, as far as possible, the ability for isolating any suspicious (diabolic or avoided crossing) points ⁽¹⁶⁾. In other words, within the numerical accuracy of 10^{-6} for individual quasicrossings, there are strong indications for singular curve (diabolic or avoided-crossings curves) configuration in the parameter space. This conclusion is supported by simple analytic arguments. In fact, it is clear that in small neighborhood of any crossing point (for example $\lambda=0$) every energy difference $\Delta E = E_2 - E_1$ may be rewritten in the following form

$$\Delta E(\vec{\lambda}) = \sqrt{(\vec{T} \cdot \vec{\lambda})^2 + (\vec{S} \cdot \vec{\lambda})^2}, \quad (\vec{\lambda} = (b, c)), \quad (11)$$

where

$$\vec{S}(0) = 2\nabla_{\lambda} H_{12}(\vec{\lambda}), \quad \vec{T}(0) = \nabla_{\lambda} [H_{11}(\lambda) - H_{22}(\lambda)]. \quad (12)$$

Therefore the exact crossing necessarily implies parallel or

antiparallel vectors \vec{S} and \vec{T} and hence defines locally direction λ orthogonal to \vec{S} (or \vec{T}). Besides that one sees the wave functions exchange by passing across this direction. The necessary condition $\vec{S} \perp \vec{T}$ has been verified numerically by over than 0.3% for levels (1,2,3 on Fig.8) in regular domain, whilst for "irregular" levels (say 3,4,5 on Fig.8) the check gives us rather bad percentage. These observations appeal to implication of fundamental topological arguments in analysis of the wave functions continued to the complex parameter space. (17)

5. Resuming all we must emphasize some common trends following from our investigations. Namely, it is very plausible hypothesis that one of the most important quantum manifestation of the classical stochasticity is the multiple quasi-crossings of levels having even non-isolated characters provided that the restrictive conditions (11) is being satisfied. Moreover these crossings are to be tightly related to : i) the destruction of shell structure under the growth of the nonintegrable perturbation ; ii) the fail of the quasiclassical energy spectral approximations ..

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