GEOMETRICAL APPROACH FOR DESCRIPTION OF THE MIXED STATE IN MULTI-WELL POTENTIALS

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We use the so-called geometrical approach [1] in description of transition from regular motion to chaotic one in Hamiltonian systems with potential energy surface that has several local minima. Distinctive feature of such systems is coexistence of different types of dynamics (regular or chaotic) in different wells at the same energy [2]. Application of traditional criteria for transition to chaos (resonance overlap criterion, negative curvature criterion and stochastic layer destruction criterion) is inefficient in case of potentials with complex topology. Geometrical approach allows considering only configuration space but not phase space when investigating the stability. In this approach all information about chaos and regularity is contained in potential function. The aim of this work is to determine what details of geometry of potential lead to chaos in Hamiltonian systems using geometrical approach. Numerical calculations are executed for potentials that are relevant with lowest umbilical catastrophes.

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1. MIXED STATE. PHENOMENOLOGICAL DESCRIPTION

Hamiltonian system with multi-well potential energy surface (PES) represents a realistic model, describing the dynamics of transition between different equilibrium states, including such important cases as chemical reactions, nuclear fission and phase transitions.

It became known in 80-th that existence of mixed state is an important feature of such systems [2]. Mixed state means that there are different dynamical regimes in different local minima at the same energy, either regular, or chaotic. For example let's demonstrate the existence of mixed state for nuclear quadrupole oscillations Hamiltonian.

It can be shown that using only transformation properties of the interaction the deformation potential of surface quadrupole oscillations of nuclei takes on the form [4]:

$$U(a_0,a_2)=\sum_{m,n} C_{mn}(a_0^2+2a_2^2)^m a_0^n(6a_2^2-a_0^2)^n\ , \quad (1)$$

where a_0 and a_2 are internal coordinates of the nuclar surface during the quadrupole oscillations:

$$R(\theta,\varphi)=R_0\{1+a_0Y_{2,0}(\theta,\varphi) +a_2[Y_{2,2}(\theta,\varphi)+Y_{2,-2}(\theta,\varphi)]\}. \quad (2)$$

Constants C_{mn} can be considered as phenomenological parameters. Restricting with the terms of the fourth degree in the deformation and assuming the equality of mass parameters for two independent directions, we get C_{3v}-symmetric Hamiltonian:

$$H=(p_x^2+p_y^2)/2m+U_{QO}(x,y;a,b,c), \quad (3)$$

where

$$U_{QO}(x,y;a,b,c) =\frac{a}{2}(x^2+y^2)+b(x^2y-\frac{1}{3}y^3)+c(x^2+y^2)^2, \quad (4)$$
$$x=\sqrt{2}a_2, y=a_0, a=2C_{10}, b=3C_{01}, c=C_{20}.$$

Hamiltonian (3) and corresponding equations of motion depend only on parameter $W=b^2/ac$, the unique dimensionless quantity we can build from parameters a,b,c. The same parameter determines the geometry of PES. Interval $0<W\le 16$ includes potentials with single extremum – minimum in the origin that corresponds to spherical symmetric shape of the nucleus. In the interval $W>16$ PES U_{QO} contains seven extrema: four minima (central, placed in the origin and three peripheral, which correspond to deformed states of nuclei) and three saddles, which separate peripheral minima from central one. The distinctive feature of transition from regularity to chaos in such a potential lies in the fact that energy of transition is not the same in different local minima. Thus, $E_{cr}\sim E_s/2$ (E_s – energy in the saddles) for the central minimum and $E_{cr}\sim E_s$ for peripheral. Due to this in the interval $E_s/2<E<E_s$ classical dynamics is mainly chaotic in the central minimum and remains regular in peripheral minima (Fig. 1). Term "mixed state" is used for designation of such specific dynamics.

Mixed state is natural for multi-well potentials. This statement is illustrated by Fig.1, which represents level lines and Poincaré sections in different energies for multi-well potentials from family of umbilical catastrophes D_5 and D_7:

$$U_{D_7}=\sqrt{2}y^2+\frac{3}{8}x^2+xy^2-\frac{1}{2}x^4+\frac{1}{6}x^6,$$
$$U_{D_5}=2y^2-x^2+xy^2+\frac{1}{4}x^4. \quad (5)$$

One can see that there exists chaos in wells with three saddles, while in other wells motion is regular.

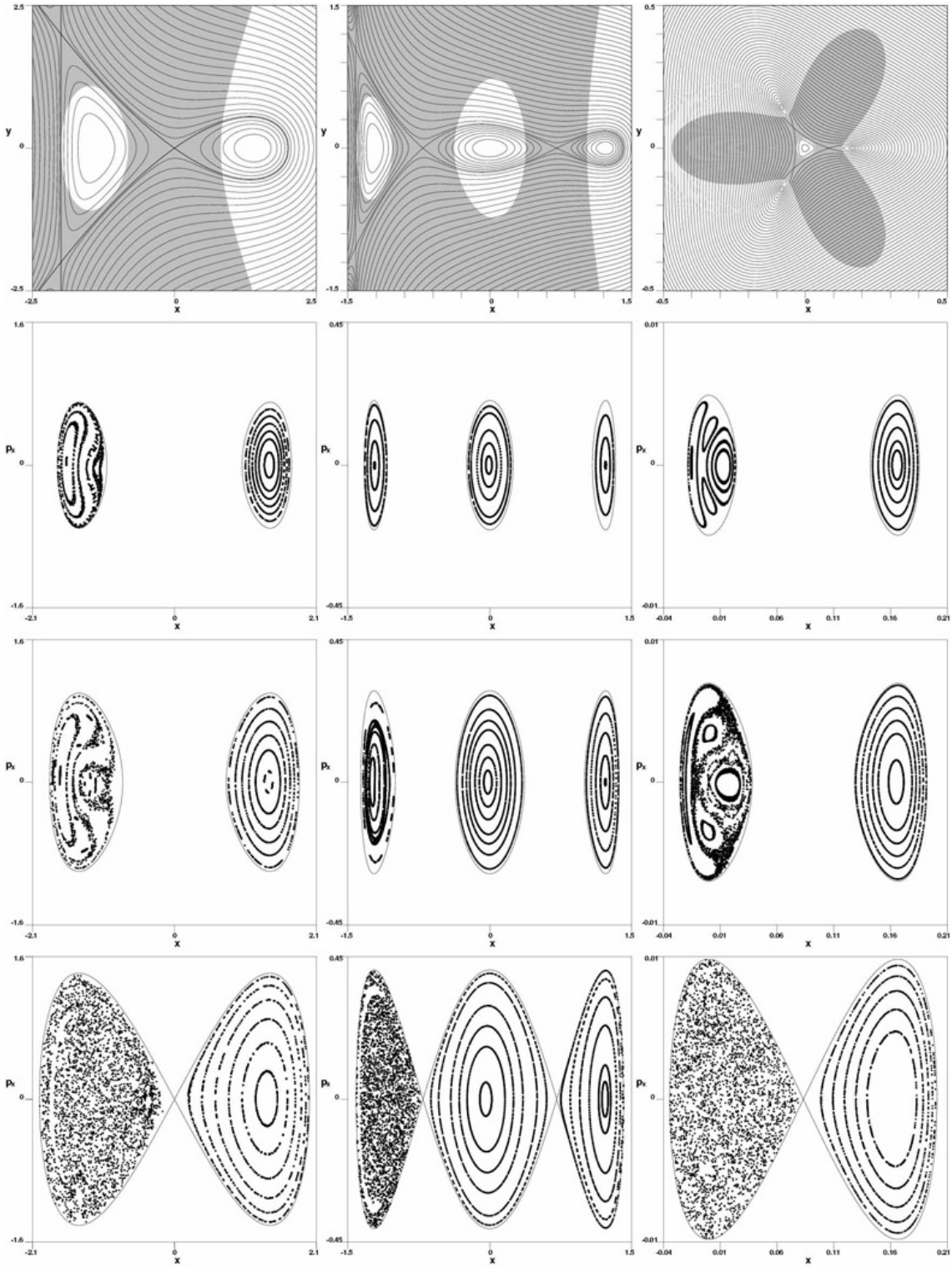

Fig. 1. *Level lines and Poincaré sections for* D_5 *(left),* D_7 *(center) and* U_{QO} *(right). Sections are presented at energies* $E_s/4$, $E_s/2$ *and* E_s

Let's note the distinction of sections structure in different wells. At the lowest energy there exists a hyperbolic point in the section for wells with chaotic motion. At the same time there is no such a point in the regular wells and structure of sections is similar at the different energies.

2. IMPORTANCE OF THE MIXED STATE FOR QUANTUM CHAOS

The mixed state represents optimal object for investigation of quantum manifestations of classical stochasticity (QMCS) in wave function structure. Indeed, usual procedure of search for QMCS in wave functions implies distinction in its structure below and above classi-

cal critical energy (or other parameters of regularity-chaos transition). However, such procedure meets difficulties connected with necessity to separate QMCS from modifications of wave functions structure due to trivial changes of its quantum numbers. Wave functions of the mixed state allow finding QMCS in comparison not different eigenfunctions, but different parts of the same eigenfunction, situated in different regions of configuration space (different local minima of the potential).

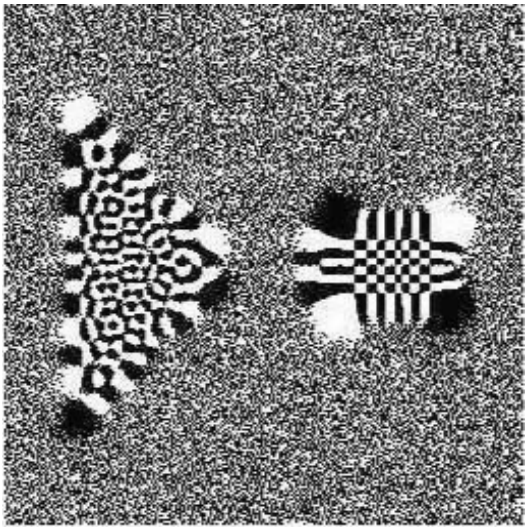

Fig. 2. *Wave function structure in D_5 potential*

For example, comparing the structure of the eigenfunctions in central and peripheral minima of the QO potential or in left and right minima of the D_5, it is evident that nodal structure of the regular and chaotic parts is clearly different, but correlating with the character of the classical motion (see Fig. 2).

3. STOCHASTIC CRITERIA FOR THE MIXED STATE

As is well known [5], stochasticity is understood as a rise of statistical properties in purely deterministic system due to local instability. According to this idea values of parameters of dynamical system, under which local instability arises, are identified as regularity-chaos transition values. However, stochasticity criteria of such a type are not sufficient (their necessity offers a separate and complicated question), since loss of stability could lead to transformation of one kind of regular motion to another one. Regardless this serious limitation, stochastic criteria in combination with numerical experiments facilitate the analysis of motion and essentially extend efficiency of numerical calculations.

The first among widely used stochasticity criteria is nonlinear resonances overlap criterion presented by Chirikov [6]. According to this criterion rise of local instability is generated by contact of separatrices of neighboring nonlinear resonances. In this approach the scenario of stochasticity is the following. The averaged motion of the system in the neighborhood of the isolated nonlinear resonance on the plane of the action-angle variables is similar to the particle behavior in the potential well. Several resonances correspond to several potential wells. The overlap of the resonances is responsible for the possibility of the random walk of particle between these wells. This method could be modified for the systems with unique resonance [7]. In this case the origin of the large-scale stochasticity is connected with the destruction of the stochastic layer near the separatrix of the isolated resonance.

Application of these criteria in presence of strong nonlinearity (which is inevitable when considering multi-well potentials) encounters an obstacle: action-angle variables effectively work only in neighborhood of local minimum. Because of this, the interest to methods, based on direct estimation of trajectories divergence speed, arises. The criterion of such a type is so-called negative curvature criterion (NCC) [8]. This criterion connects stochastisation of motion with getting to part of configuration space, where Gaussian curvature of PES is negative when energy increases (while in neighborhood of minima curvature is always positive). Then energy of transition to chaos is close to minimal energy on the zero-curvature line. However, when passing on to the multi-well potentials, NCC fails to work correct. In particular, for above mentioned potentials (D_5 and D_7), structure of Gaussian curvature is similar in different wells. For example, for D_5 potential according to NCC we get the same value of critical energy for both minima: *-5/9*, but chaotic motion is observed only in the left well (see Fig. 1). A natural question immediately arises: is it possible to formulate, using only geometrical properties of PES but not solving numerically equations of motion, the algorithm for finding the critical energy for single local minima in multi-well potential? We'll try to answer this question below in the framework of geometrical approach.

4. GEOMETRICAL APPROACH TO HAMILTONIAN MECHANICS

We will use so-called geometrical approach in consideration of mixed state [1]. Let's recall the basics of this method.

It is known that Hamiltonian dynamics could be formulated in the terms of Riemannian geometry. In this approach trajectories of the system are considered as geodesics of some manifold. Grounds for such consideration lie in variational base of Hamiltonian mechanics.

Geodesics are determined by condition:

$$\delta \int_L ds = 0 . \tag{6}$$

At the same time trajectories of dynamical system are determined according to the Maupertuis principle:

$$\delta \int_\gamma 2T dt = 0 \tag{7}$$

(γ are all isoenergetic paths connecting end points) or to the Hamilton's principle:

$$\delta \int_{t_1}^{t_2} L dt = 0 . \tag{8}$$

Once chosen a suitable metric action could be rewrote as a length of the curve on the manifold. Then

trajectories will be geodesics on this manifold. This approach has an evident advantage: potential energy function includes all information about the system, so one needs to consider only configuration space but not phase space.

Equations of motion in this case take on the form:

$$\frac{d^2q^i}{ds^2} + \Gamma^i_{jk}\frac{dq^j}{ds}\frac{dq^k}{ds} = 0\,. \tag{9}$$

Christoffel symbols in this approach play role of counterparts of forces in ordinary mechanics.

The most natural metric is the Jacobi one. It has the form:

$$g_{ij} = 2[E - V(q)]\delta_{ij}\,. \tag{10}$$

By means of this metric Maupertuis principle could be rewritten in the form equivalent to condition for geodesics.

Let's consider local instability in the framework of above mentioned geometrical approach. Let q and $q`$ be two trajectories, close at $t=0$:

$$q^{`i}(s) = q^i(s) + J^i(s)\,. \tag{11}$$

Separation vector then satisfy the Jacobi-Levi-Civita equation:

$$\frac{d^2J^i}{ds^2} + R^i_{jkl}\frac{dq^j}{ds}J^k\frac{dq^l}{ds} = 0\,. \tag{12}$$

It can be shown that dynamics of the deviation is determined only by Riemannian curvature of the manifold. For two-degrees-of-freedom systems Riemannian curvature has the form:

$$R = \frac{1}{4(E-V)^2}[2(E-V)\Delta V + 2|\nabla V|^2]\,. \tag{13}$$

Laplacian of V is positive for considered potentials so Riemannian curvature is positive too. Due to this we couldn't connect divergence of trajectories with negative Riemannian curvature.

One way to solve this problem consists in introduction of higher-dimensional (than N) metrics. Let's examine this question closer.

It can be shown that equation for separation vector J could be reformulated in the form, which doesn't depend on dimensionality of manifold:

$$\frac{1}{2}\frac{d^2\|\vec{J}\|^2}{ds^2} + K^{(2)}(\vec{J},\vec{v})\|\vec{J}\|^2 - \left\|\frac{\nabla}{ds}\vec{J}\right\|^2 = 0\,, \tag{14}$$

where $K^{(2)}$ is a sectional curvature in two-dimensional direction:

$$K^{(2)}(\vec{J},\vec{v}) = R_{iklm}\frac{J^i}{\|\vec{J}\|}\frac{dq^k}{ds}\frac{J^l}{\|\vec{J}\|}\frac{dq^m}{ds} \tag{15}$$

and $\left\langle \vec{J},\vec{v}\right\rangle = 0$.

Note that the point where $K^{(2)}<0$ is unstable. Since there are more than one sectional curvature for the case $N>2$, we could connect instability with negative sign of some of them.

One of the enlarged metrics is the Eisenhart metric. Eisenhart metric is $N+2$-dimentional and contains two additional coordinates. One of these coordinates coincides with time and second is connected with action. Using Eisenhart metric, quantity $K^{(2)}$ could be rewritten in the form:

$$K^{(2)}(\dot{\vec{q}},\vec{q}) = \frac{1}{2(E-V)}\left(\frac{\partial^2V}{\partial q_1^2}\dot{q}_2^2 + \frac{\partial^2V}{\partial q_2^2}\dot{q}_1^2 - 2\frac{\partial^2V}{\partial q_1\partial q_2}\dot{q}_1\dot{q}_2\right). \tag{16}$$

Now, investigation the $K^{(2)}$-structure on the considered manifold could be used for studying the chaotic regimes and, in particular, the mixed state.

Let's briefly summarize the basics of geometrical approach to Hamiltonian mechanics:

dynamics ~	geometry
t (time) ~	s (arc-length)
V (potential energy) ~	g (metric)
∂V (forces) ~	Γ (Christoffel symbols)
$\partial^2 V$, $(\partial V)^2$ (curvature of potential) ~	R (curvature of potential)

5. INVESTIGATION OF THE MIXED STATE IN THE FRAMEWORK OF GEOMETRICAL APPROACH

As mentioned above, negative sign of $K^{(2)}$ is a condition for rise of local instability. It is necessary to clarify whether this condition is sufficient for development of chaoticity or not, clearly speaking, one needs to answer the question: does the presence of negative curvature parts on CM always lead to chaos? Potentials with mixed state represent a very convenient model for investigation of this question, since there exist both regimes of motion.

So, we need to study, how differs the structure of $K^{(2)}$ in different wells. For that we calculate the fraction of phase space with negative curvature as a function of energy, i.e. a volume of phase space where $K^{(2)}<0$ referred to the total volume:

$$\mu(E) = \frac{\int d\vec{q}d\vec{p}\,\Theta(-K^{(2)})\delta(H(\vec{q},\vec{p}) - E)}{\int d\vec{q}d\vec{p}\,\delta(H(\vec{q},\vec{p}) - E)}\,. \tag{17}$$

An advantage of this approach consists in necessity to calculate only geometrical properties of system without solving equations of motion.

We carried out calculations for two potentials: D_5 and D_7.

Calculations of μ (Fig. 3) show that there are regions, where $K^{(2)}<0$, in all wells, but nevertheless chaos exists only in one well. Moreover, for the well with chaotic motion function $\mu(E)$ gives correct value of critical energy (in the sense, specified in part 3). At this energy μ becomes positive.

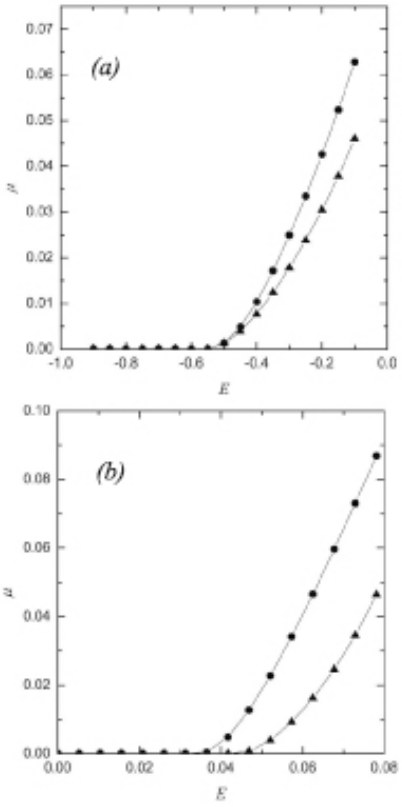

Fig. 3. *Function μ(E) for D_5 (a) and D_7 (b) potentials. Data for chaotic wells are represented by circles, for regular – by triangles*

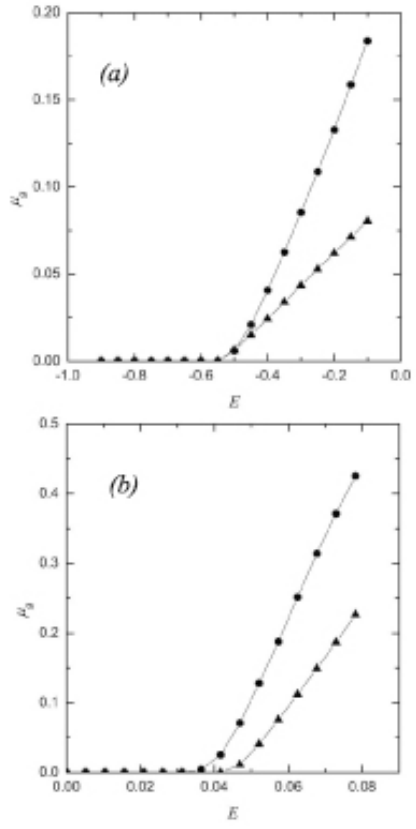

Fig.4. *Function μ_g (E) for D_5 (a) and D_7 (b)*

Situation with regular wells is more complicated. Although the fraction of phase space, where $K^{(2)} < 0$, is nonzero, chaos in the well doesn't exist. This can be seen on the Poincaré sections. For comparison the fraction of CS with negative Gaussian curvature is shown in Fig. 4. One can see that structure of negative Gaussian curvature is similar to the $K^{(2)}$-structure. To understand this similarity let's introduce polar coordinates in space of momenta. $K^{(2)}$ then becomes:

$$K^{(2)}(\vec{q},\varphi) = \frac{\partial^2 V}{\partial q_1^2}(\sin\varphi)^2 + \frac{\partial^2 V}{\partial q_2^2}(\cos\varphi)^2 - 2\frac{\partial^2 V}{\partial q_1 \partial q_2}\cos\varphi \sin\varphi, \quad (18)$$

where φ is the polar angle. Evidently $K^{(2)}$ could be negative only if Gaussian curvature is negative.

6. CONCLUSIONS

Investigation of curvature of manifold, as one can see from the cited above data, doesn't give a plain method for identification of chaos in any minimum, especially if there exist both regular and chaotic regimes of motion. It is impossible to determine a priori whether chaos exists in the system without using the dynamical description (in our case that are Poincaré sections). Nevertheless, one can efficiently use geometrical methods for investigation of chaos in multi-well potentials.

In above considered potentials chaos exists only in wells, which have two details: non-zero fraction of negative curvature on the manifold and at least one hyperbolic point in the Poincaré section. According to this, one can use the following method for identification of chaos and calculation of critical energy. At the first step the Poincaré section in low energy is drown for the well and the presence of hyperbolic point is determined. If so, the quantity μ must be calculated (or the fraction of CS with negative Gaussian curvature). Value of energy, in which μ becomes positive, could be associated with critical energy. If there is no hyperbolic point in the section than chaos doesn't exist in the well.

Consequently, geometrical methods could be efficiently used for determination of critical energy in complicated potentials and identification of chaos in general. However, one must carefully use these methods and combine them with qualitative methods, such as Poincaré sectioning method.

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ГЕОМЕТРИЧЕСКИЙ ПОДХОД К ОПИСАНИЮ СМЕШАННОГО СОСТОЯНИЯ В МНОГОЯМНЫХ ПОТЕНЦИАЛАХ

В.П. Березовой, Ю.Л. Болотин, Г.И. Ивашкевич

Мы используем так называемый геометрический подход [1] в описании перехода от регулярного движения к хаотическому в гамильтоновых системах, в которых поверхность потенциальной энергии имеет несколько локальных минимумов. Отличительная черта таких систем – сосуществование различных типов динамики (регулярного или хаотического) в разных потенциальных ямах при той же самой энергии [2]. Применение традиционных критериев для перехода к хаосу (критерий перекрытия резонансов, критерий отрицательной кривизны и критерий разрушения стохастического слоя) неэффективно в случае потенциалов с комплексной топологией. Геометрический подход при исследовании устойчивости позволяет рассматривать только пространство конфигураций, но не фазовое пространство. В этом подходе вся информация относительно хаоса и регулярности содержится в потенциальной функции. Цель настоящей работы состоит в том, чтобы, используя геометрический подход, определить какие детали геометрии потенциала приводят к хаосу в гамильтоновых системах. Численные расчеты выполнены для потенциалов, которые соответствуют самым низким омбилическим катастрофам.

ГЕОМЕТРИЧНИЙ ПІДХІД ДО ОПИСУ ЗМІШАНОГО СТАНУ У БАГАТОЯМНИХ ПОТЕНЦІАЛАХ

В.П. Березовий, Ю.Л. Болотін, Г.І. Івашкевич

Ми використовуємо так званий геометричний підхід [1] в описі переходу від регулярного руху до хаотичного в гамільтонових системах, у яких поверхня потенційної енергії має кілька локальних мінімумів. Відмітна риса таких систем – співіснування різних типів динаміки (регулярного або хаотичного) у різних потенційних ямах при тій же самій енергії [2]. Застосування традиційних критеріїв для переходу до хаосу (критерій перекриття резонансів, критерій негативної кривизни й критерій руйнування стохастичного шару) неефективно у випадку потенціалів із комплексною топологією. Геометричний підхід при дослідженні стабільності дозволяє розглядати тільки простір конфігурацій, але не фазовий простір. У цьому підході вся інформація щодо хаосу й регулярності міститься в потенційній функції. Ціль даної роботи полягає в тому, щоб, використовуючи геометричний підхід, визначити які деталі геометрії потенціалу приводять до хаосу в гамільтонових системах. Чисельні розрахунки виконані для потенціалів, які відповідають найнижчим омбілічним катастрофам.