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The measure of chaoticity in stationary quantum systems

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Abstract

Our earlier suggested quantum chaoticity measure characterizing the initial symmetry breaking and the destruction of the corresponding integrals of motion in a perturbed system is used for the analysis of the quantum Henon–Heiles Hamiltonian and diamagnetic Kepler problem. We demonstrate that the critical perturbation parameter for the transition from regularity to chaos in the quantum systems is in remarkable agreement with the classical picture of chaotization. We also show that this critical parameter can be estimated in the framework of first-order perturbation theory.

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1. Introduction

During past decades investigations of quantum chaos have been extensively carried out but this field remains a centre of discussions. There is a variety of concepts of quantum chaos and different understanding of problems in this field [1]. This essentially comes from the fact that in quantum systems there seems to be nothing similar to the well investigated classical chaos. In contrast, some attributes of 'regularity' seem to exist because of unitarity of quantum evolution. While the Lyapunov instability of the system's trajectories is believed to be the main feature of the classically chaotic system, the concept of the trajectory does not apply in quantum mechanics. For these and some other reasons, many specialists believe that quantum chaos does not exist at all, and that it is necessary to study phenomena arising in the semiclassical region, i.e. quantum 'signatures' of classical chaos [2]. However, from the theoretical point of view such an approach is not quite satisfactory since we face the obvious contradiction to the fundamental correspondence principle: the more general quantum theory does not comprise a phenomena (namely chaos) which exists in its classical limit [3].

Therefore we tried to develop a new approach to the problem of quantum chaos which meets the following natural requirements:

- it is formulated in the universal language which is common both for classical and quantum systems;
- it allows one to construct a quantitative measure of quantum chaoticity;
- in the semiclassical limit this quantum measure transforms into the measure of chaoticity of the classical system (into the Lyapunov exponent or Kolmogorov entropy).

In section 2 we briefly reconsider our definition of the quantum chaoticity and its measure, which we then use for the investigation of the transition from regularity to chaos in the quantum Henon–Heiles system and diamagnetic Kepler problem in section 3. Section 4 is devoted to the approximate estimate of the quantum chaoticity criterion in the framework of the first-order perturbation theory. The comparison of this estimate with the exact calculations for the Henon–Heiles Hamiltonian and diamagnetic Kepler problem is performed in section 5.

2. Symmetry breaking and chaos

Our approach to the problem of quantum chaoticity [4–9] is based on the generalization of the Liouville–Arnold theorem in classical mechanics, which states that the Hamiltonian system with f degrees of freedom is regular if it has $m = f$ independent global integrals of motion. If the number m of global integrals becomes less than f, the system becomes chaotic. The well known Noether's theorem connects the existence of global integrals of the system with the symmetries of its Hamiltonian. According to this theorem, breaking the symmetry of the initially regular system decreases the number of its independent global integrals of motion. Thus the system becomes chaotic *only* in the case of such a symmetry breaking which makes the number m of global integrals *less* than f.

Our first suggestion is to generalize this definition of chaoticity for the case of quantum systems. Since the concept of symmetry (unlike the trajectory) is universal for both classical and quantum mechanics, this generalization seems to be quite straightforward—one should simply substitute the integrals of motion by the corresponding 'good' quantum numbers, resulting from the symmetries of quantum Hamiltonian. Our second suggestion is to use the concept of spreading width Γ_{spr} (and the related parameter æ) as a sensitive measure of symmetry breaking of the Hamiltonian H_0 caused by the perturbation λV. This idea is borrowed from the 'strength function' phenomenon in nuclear physics (see e.g. ch 2 of [10]) which served the most important indication that the symmetry traces of the regular independent-particle motion in the nuclear mean field survive in spite of the strong pair-wise nucleon–nucleon forces, which tend to destroy this symmetry. Indeed, consider a Hamiltonian H of the non-integrable system as a sum

$$H = H_0 + \lambda V \tag{1}$$

of the highly symmetrical integrable Hamiltonian H_0

$$H_0\phi_k = \epsilon_k\phi_k \tag{2}$$

and of the perturbation λV which destroys a symmetry of H_0 and reduces the number of 'good' quantum numbers to $m < f$. Expand now the eigenstates ψ_i of H over the 'regular' basis $\{\phi_k\}$:

$$\psi_i = \sum_k \langle\phi_k|\psi_i\rangle\phi_k = \sum_k c_i^k\phi_k \tag{3}$$

and look for the probability $P_k(E_i) = |c_i^k|^2$ of finding the original 'regular' component ϕ_k in the different eigenstates ψ_i (with eigenenergies E_i) of our nonintegrable system. It is known that for sufficiently small λ this probability would be localized in rather narrow energy

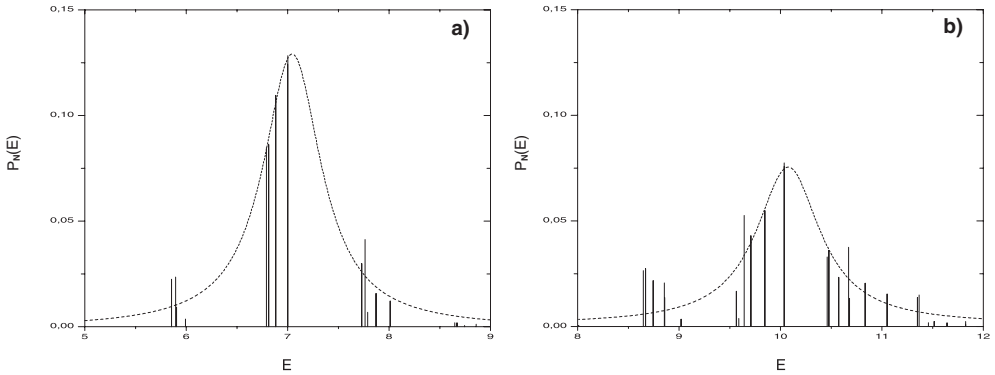

Figure 1. Probability distribution $P_N(E)$ for (*a*) $N = 6$ and (*b*) $N = 9$ for the Henon–Heiles Hamiltonian. The dashed curves are the Lorentz distributions with the values of Γ^N_{spr} calculated as pointed out in the text.

intervals in the vicinity of the 'initial' eigenvalues ϵ_k. The Hamiltonian H diagonalization under rather general realistic assumptions (see e.g. appendix 2D of [10] in the nuclear many-body case or figure 1 of this paper for the Henon–Heiles problem) shows that the strength function $S_k(E_i) \sim P_k(E_i)$ energy dependence can be approximated by the Lorentzian-type distribution:

$$S_k(E_i) = \frac{|c_i^k|^2}{D} \approx \frac{1}{2\pi} \frac{\Gamma^k_{spr}}{(E_i - \epsilon_k)^2 + (\Gamma^k_{spr})^2/4} \tag{4}$$

where D is the average level spacing of the nonintegrable system and Γ^k_{spr} characterizes the coupling of the state ϕ_k to other 'unperturbed' states caused by the perturbation λV.

Keeping this in mind let us define the energy spreading width Γ^k_{spr} of the $P_k(E_i)$ distribution as the minimal energy interval around the distribution maximum where the sum of probabilities $\sum_i P_k(E_i)$ is equal to 0.5. Thus Γ^k_{spr} is defined for each of the basis states ϕ_k. We want to find a parameter characterizing the measure of the initial symmetry breaking of H_0 under the influence of the perturbation λV. If the spreading width Γ^k_{spr} is smaller than the distance D_0 between the maxima of the adjacent distributions $P_k(E_i)$ we can distinguish the 'localization domain' (in energy) of one basis state (with a given principal quantum number) from the 'localization domain' of another one. Thus, although formally the initial symmetry is broken by the perturbation, its traces are still visible as isolated maxima of the $P_k(E_i)$ distribution. When the spreading width exceeds D_0 we start losing the 'traces' of the basis functions in the spectrum of H and cannot even approximately connect states ψ_i with the basis states ϕ_k. Thus a dimensionless parameter [4]

$$æ^k = \Gamma^k_{spr}/D_0 \tag{5}$$

is the natural measure of the symmetry breaking. When the parameter $æ^k$ exceeds unity the symmetry 'traces' of the Hamiltonian H_0 disappear. Such a value of perturbation is accompanied by the disappearance of the initial selection rules, the levels are distributed approximately uniformly (level repulsion) and the level spacing distribution approaches Wigner's law. For these and other reasons one can say that the onset of chaoticity has taken place in the quantum system and $æ^k$ may be considered as the quantitative measure of chaoticity [5,6].

The spectrum of H_0 may be degenerate and then the irreducible representations $\mathcal{T}_N$ of the symmetry group of H_0 consist of several basis functions which belong to one energy level (shell) with the principal quantum number N. To generalize our considerations to the degenerate case we should take into account that symmetry breaking results only due to the

mixing between functions from different irreducible representations. Thus, in the general case we should consider the following distribution:

$$P_N(E_i) = \frac{1}{\dim \mathcal{T}_N} \sum_{k \in \mathcal{T}_N} |\langle \phi_k | \psi_i \rangle|^2 \tag{6}$$

and determine its energy width Γ^N_{spr}:

$$\Gamma^N_{spr} = \min \left\{ \Delta E \middle| \sum_{E_i \in \Delta E} P_N(E_i) = 0.5 \right\} \tag{7}$$

where $\mathcal{T}_N$ is a degenerate level subspace ($\dim \mathcal{T}_N$ means its dimension) with the principal quantum number N. The 'averaged' parameter Γ^N_{spr} (and $P_N(E_i)$) has an important property of invariance with respect to the choice of the basis for the integrable Hamiltonian H_0 [8].

From the theoretical point of view the above chaoticity measure has one more very important property. It can be shown [5] that $\Gamma^k_{spr}/\hbar$ defines the rate of decay of the 'regular' states ϕ_k resulting from the instability caused by the perturbation λV. This can be easily shown in terms of the non-stationary formalism of quantum mechanics. Suppose that, at the initial instant $t = 0$, a wavepacket formed by the eigenstates of the total Hamiltonian H is created in such a way that it describes the particular eigenstate ϕ_k of the unperturbed Hamiltonian H_0:

$$\phi_k(t = 0) = \sum_i (c^k_i)^* \psi_i(t = 0). \tag{8}$$

Let us find the survival probability of this state

$$P(t) = |\langle \phi_k(0) | \phi_k(t) \rangle|^2 \equiv |A(t)|^2$$

in the perturbed system. Considering that the functions ψ_i are orthogonal and making use of (4), we can estimate the correlation function $A(t)$ (see [10]):

$$\begin{aligned} A(t) = \langle \phi_k(0) | \phi_k(t) \rangle &= \sum_i |c^k_i(E_i)|^2 \exp\left(-\frac{\mathrm{i} E_i t}{\hbar}\right) \\ &\approx \int \frac{\mathrm{d}E_i}{D} |c^k_i(E_i)|^2 \exp\left(-\frac{\mathrm{i} E_i t}{\hbar}\right) \\ &= \int \frac{\mathrm{d}E_i}{2\pi} \frac{\Gamma^k_{spr}}{(E_i - \epsilon_k)^2 + (\Gamma^k_{spr})^2/4} \exp\left(-\frac{\mathrm{i} E_i t}{\hbar}\right) \\ &= \exp\left(-\frac{\Gamma^k_{spr}}{2\hbar} t - \mathrm{i} \frac{\epsilon_k t}{\hbar}\right). \end{aligned} \tag{9}$$

Therefore

$$P(t) = \exp\left(-\frac{\Gamma^k_{spr}}{\hbar} t\right). \tag{10}$$

Thus the damping of the quasiparticle motion in the quantum many-body system is defined by the spreading width Γ_{spr}. The simplest way to allow for this damping in nuclear physics is given by the optical model where the imaginary part $W = 2\Gamma_{spr}$ is added to the mean field potential (see e.g. [10]). In terms of the more refined Green function approach to the many-body theory W is approximately the imaginary part of the self-energy operator (see, e.g., [11]).

In order to find the classical limit of Γ_{spr} one can use [4–6] the results of Heller's experience (see e.g. [14, 15] or paragraph 15.6 of [16]) with Gaussian wavepackets $|\Phi\rangle$. Heller launched such a packet in such a way that at the initial moment $t = 0$ its centre moved along the periodic trajectory with period T and calculated the recurrence probabilities $P_\Phi(t) = |\langle \Phi(0) | \Phi(t) \rangle|^2$.

He showed that, in the semiclassical limit, this probability developed the periodically repeated maxima with period T, which correspond to the returns of the wavepacket in the initial element of the phase space. However, the amplitudes of these maxima were modulated by the factor $\exp(-\frac{\Lambda t}{2})$, where Λ is the classical Lyapunov exponent. The reduction of the probability $P(t)$ for two successive returns was

$$\mathrm{e}^{-\Lambda T} = \mathrm{e}^{-\chi}.$$

In classical mechanics the dimensionless quantity $\chi = \Lambda T$ is referred to as (see, e.g., [16]) a stability parameter for the monodromy matrix.

Following Heller, we can construct the wavepacket

$$|\Phi(t)\rangle = \sum_n A_n |\phi_n(t)\rangle \tag{11}$$

where each of the functions $\phi_n(t)$ is represented by (8). Just for the sake of simplicity we can choose the potential of the regular Hamiltonian H_0 to be a one-dimensional harmonic oscillator with potential $m\omega^2 x^2/2$ (more complicated potentials would simply demand cumbersome numerical computations without clarifying the main physical results). In this case we shall have at $t = 0$ the Gaussian wavepacket

$$|\Phi(t=0)\rangle = \frac{1}{(\pi)^{1/4}\sqrt{\sigma}} \exp\left[-\frac{(x-a)^2}{2\sigma^2}\right] \tag{12}$$

while the coefficients in (11) would be (see [12])

$$A_n = \left(\frac{a}{\sigma}\right)^n \frac{\mathrm{e}^{-(a/2\sigma)^2}}{\sqrt{2^n n!}} \tag{13}$$

where $\sigma = \sqrt{\hbar/m\omega}$ and a are, respectively, the localization spread and the initial displacement of the packet. Substituting now expansion (11) into the correlation function $\langle\Phi(0)|\Phi(t)\rangle$ we obtain

$$\langle\Phi(0)|\Phi(t)\rangle = \sum_n |A_n|^2 \langle\phi_n(0)|\phi_n(t)\rangle + \sum_{m\neq n} A_n^* A_m \langle\phi_n(0)|\phi_m(t)\rangle. \tag{14}$$

For small times $t \lesssim \hbar/\Gamma_{spr}$ the double sum in this expression can be neglected because of the approximate orthogonality of the functions $\phi_n(0)$ and $\phi_m(t)$ (note that the exponential decay in the approximate expression (9) holds also for small $\Gamma_{spr}t/\hbar \lesssim 1$—see, e.g., [13]). Therefore making use of (13) and (9) we obtain for the recurrence probability

$$P_\Phi(t) = |\langle\Phi(0)|\Phi(t)\rangle|^2 = \exp\left[a^2(\cos\omega t - 1)/\sigma^2\right] \exp\left[-\Gamma_{spr}t/\hbar\right]. \tag{15}$$

The first factor here describes the periodic returns of the packet with oscillator frequency ω, while the second factor demonstrates the reduction of the recurrence probability due to the instability of the trajectory (in the nuclear case this damping is caused by the coupling of the single-particle mode to the more complex modes). In the classical limit Γ_{spr} in this expression corresponds to the energy of the classical oscillator with amplitude a.

Comparing our results of (15) with the above results of Heller, we conclude that the quantity $\Gamma_{spr}/\hbar$ transforms in the classical limit into the Lyapunov exponent Λ:

$$\frac{\Gamma_{spr}}{\hbar} \to \Lambda. \tag{16}$$

The corresponding classical limit for the dimensionless chaoticity measure is

$$æ \to \frac{\Lambda T}{2\pi} = \frac{\chi}{2\pi} \tag{17}$$

where T is the classical period and χ is the stability parameter of the classical monodromy matrix.

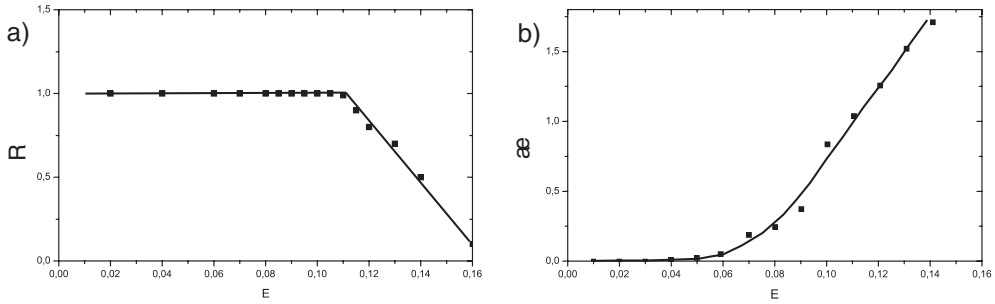

Figure 2. Classical (a) and quantum (b) measures of chaoticity for the Henon–Heiles Hamiltonian.

3. Tests of the quantum chaoticity criterion

In order to check the validity of the above approach we examined the two most popular 'textbook' examples of transitions from regularity to chaos in classical systems. One of them was the Henon–Heiles system—a two-dimensional harmonic oscillator perturbed by the nonlinear terms where the excellent agreement with classical picture of chaotization was found [7]. Here we review briefly this result for completeness. The classical Henon–Heiles Hamiltonian is

$$H(q,\,p) = \tfrac{1}{2}(p_x^2 + x^2) + \tfrac{1}{2}(p_y^2 + y^2) + \lambda(x^2 y - y^3/3) = H_0 + \lambda V \tag{18}$$

where H_0 is the Hamiltonian of the two-dimensional harmonic oscillator (we use the standard choice of $\omega = m = 1$) and V is the perturbation. For the 'standard' choice $\lambda = 1$ the motion is bounded up to separation energy $E_s = 1/6$. Henon and Heiles [17] investigated a portion R of the phase portrait area covered by the regular trajectories as a function of energy (figure 2(a)) and found that up to the critical energy $E_{cr} = 0.11$ this portion is very close to unity. For higher energies $E > E_{cr}$ this portion goes down giving way to the increasing domains covered by the stochastic trajectories. Their conclusion was: 'the situation can be very roughly described by saying that the second integral exists for orbits below a critical energy E_{cr} and does not exist for orbits above that energy'.

The quantum Henon–Heiles Hamiltonian is obtained by substituting the momenta in equation (18) with the corresponding momentum operators. As is well known, the two-dimensional harmonic oscillator Hamiltonian H_0 has $SU(2)$ symmetry. It is easy to write out matrix elements of the Hamiltonian (18) in the oscillator basis $\phi_{n_x n_y}$ and to find through a diagonalization the system's eigenenergies E_i and eigenstates ψ_i in terms of the expansion coefficients c_i^k (see equation (3)). In our calculations the values $\lambda = 1$ and $\hbar = 0.01$ were fixed (in this case about 150 levels (16 shells) are bounded) and 496 basis functions were used. As a next step, we calculated the energy distributions $P_N(E_i)$ (6) for $N = 1, \ldots, 15$ and found their energy spreading widths Γ_{spr}^N. Figures 1(a) and (b) show the example of the distributions for $N = 6$ and 12, respectively. Thus obtained values of Γ_{spr}^N were divided then by the spacing D_0 between the maxima of the adjacent $P_N(E_i)$ to give the desired parameter æ. The plot of this parameter as a function of the energy E is given in figure 2(b).

We see that our parameter reaches the critical value of æ $= 1$ at the critical energy $E = 0.11$. Paraphrasing Henon and Heiles, the situation now can be roughly described by saying that oscillator symmetry in the quantum case exists for energies below the critical $E_c = 0.11$ and disappears above it. This remarkable agreement between the classical and the quantum pictures already indicates that our parameter æ indeed might serve as a quantitative measure of chaoticity.

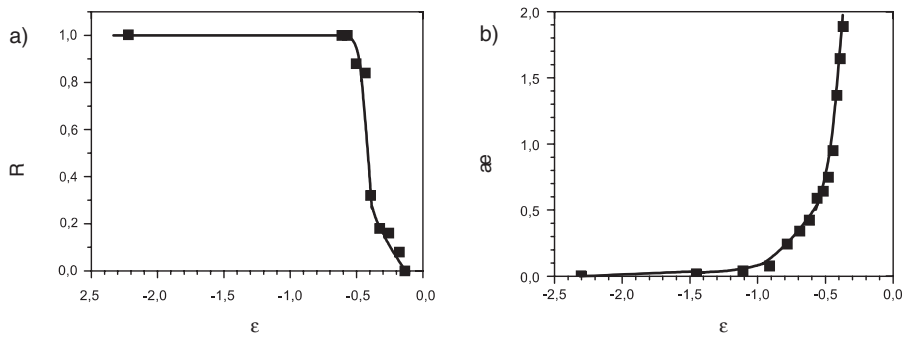

Figure 3. Classical (*a*) and quantum (*b*) measures of chaoticity for the diamagnetic Kepler problem.

Another very popular model for the studies of transition from regularity to chaos in classical mechanics is the non-relativistic hydrogen atom in the uniform magnetic field described by the Hamiltonian

$$H = p^2/2m - e^2/r + \omega l_z + \tfrac{1}{2}m\omega^2(x^2 + y^2). \tag{19}$$

Here the frequency $\omega = eB/2mc$ is a half of the cyclotron frequency and B is the strength of the magnetic field acting along the z-axis. The dimensionless field strength parameter $\gamma = \hbar\omega/\mathcal{R}$ (here $\mathcal{R}$ is the Rydberg energy) is usually combined with the electron energy E to produce the scaled energy $\epsilon = E\gamma^{-2/3}$. The fraction R of available phase space covered by regular trajectories was calculated in [18, 19] as a function of scaled energy for the case of $l_z = 0$ (see figure 3(*a*)), showing the rapid chaotization of the system in the range $-0.48 \leqslant \epsilon \leqslant -0.125$.

We analysed the quantum analogue of this system along the same lines as it was performed for the quantum Henon–Heiles problem, namely we traced the gradual destruction of the $O(4)$ symmetry characteristic of the unperturbed motion in Coulomb potential by the external magnetic field. In other words, we traced the disappearance of the 'good' quantum numbers (integrals of motion) which characterize the regular motion in this potential. In order to do this, we diagonalized the matrix of Hamiltonian (19) in the basis of purely Coulomb wavefunctions $\phi_{n_1,n_2,m}$ with principal quantum number $N = n_1 + n_2 + |m| + 1$, and calculated the new eigenvalues E_i and the eigenstates ψ_i for various values of field strength γ. For the investigation of fragmentation of basis functions with $m = 0$ from a shell with the principal quantum number $N = 10$ we used the basis of the first 20 shells. As a next step, we calculated the energy distribution $P_N(E_i)$ (6) for the $N = 10$th shell and found its energy spreading width Γ^N_{spr}. Thus obtained values of Γ^N_{spr} were divided then by the spacing D_0 between the maxima of the adjacent $P_N(E_i)$ to give the desired parameter æ. The plot of this parameter as a function of the scaled energy ϵ is given in figure 3(*b*).

We see that our parameter reaches the value of æ $= 1$ at the critical scaled energy $\epsilon_{cr} = -0.45$ in fairly good agreement with the classical critical value $\epsilon_{cr} = -0.48$ of [18, 19].

4. The approximate estimate of the quantum chaoticity parameter

As we had already shown, the transition from regularity to chaos in quantum systems occurs at a certain critical perturbation intensity (for example, at a certain value of the parameter λ in (1)). So far, we had to diagonalize the perturbed system's Hamiltonian matrix in order to calculate this critical parameter. Now we shall show how this critical perturbation parameter can be estimated in a simpler semi-analytical way.

In order to do this we shall take into account that: (i) the expansion coefficients (3) for small parameter λ can be computed in the framework of the perturbation theory and (ii) since it is inconvenient to work with the distribution width Γ^N_{spr} analytically, we shall use the connection of our chaoticity criterion based on parameter æ with the Hose–Taylor approach.

Hose and Taylor [20,21] investigated the problem of effective Hamiltonians and suggested the criterion of their existence together with their integrals of motion. According to this criterion, one can construct a convergent sequence of approximations to the effective Hamiltonian provided that a squared projections of the perturbed wavefunction on the trial space (formed by the eigenstates of the integrable system) is larger than 0.5. Operators commuting with the effective Hamiltonian will be the approximate integrals of motions of the system considered. Thus, if the squared projections of some states ψ_i of the Hamiltonian H on the space $\mathcal{T}_N$ of the level of H_0 are larger than 0.5, then the principal quantum number must be the approximate integral of motion for these 'regular' states [20].

It is easy to connect our approach with Hose–Taylor's one. Indeed, when æ < 1 the distributions $P_N(E_i)$ are well localized and do not overlap significantly for the adjacent shells N. We can approximately attribute wavefunctions ψ_i to various irreducible representations $\mathcal{T}_N$. Let us introduce the averaged (over $i \in \mathcal{T}_N$) square of the ψ_i projection $P(\lambda, N)$ on the subspace $\mathcal{T}_N$:

$$P(\lambda, N) = \frac{1}{\dim \mathcal{T}_N} \sum_i \sum_{\alpha \in \mathcal{T}_N} |c_i^\alpha|^2$$

where i are the indices of wavefunctions ψ_i being averaged. When æ ≈ 1 we have about $\dim \mathcal{T}_N$ functions ψ_i on the localization length Γ^N_{spr} of $P_N(E_i)$ distribution and these functions in accordance with (7) saturate $0.5\ \dim \mathcal{T}_N$ of total probability. Therefore $P(\lambda, N)$ should equal 0.5 approximately for the same critical perturbation which gives æ $= 1$. This is in agreement with the above Hose–Taylor condition for the existence of the approximate integrals of motion.

The next principal problem in using the perturbation theory for estimating the squares of projections is the degeneracy of basis states and, hence, the necessity to solve a secular equation, which prevents one obtaining the analytical expressions. In order to bypass this complexity we shall act as follows. We shall construct such a quantity, which will help us to estimate the critical perturbation parameter and will be invariant with respect to the block unitary transformations inside all the subspaces $\mathcal{T}_n$. This latter property will allow us to replace in evaluating this quantity the states obtained from the secular equation, by the initial basis states ϕ_α.

Let us estimate the average square of projection $W(\lambda, N)$ of the perturbed wavefunctions not on a subspace $\mathcal{T}_N$, but on its orthogonal adjoint $\mathcal{H} \ominus \mathcal{T}_N$:

$$W(\lambda, N) = 1 - P(\lambda, N) = \frac{1}{\dim \mathcal{T}_N} \sum_i \sum_{\alpha \notin \mathcal{T}_N} |c_i^\alpha|^2 \tag{20}$$

where i are the indices of wavefunctions ψ_i being averaged. Utilizing W instead of P will allow us to use the perturbation theory since for small λ the mixture of the states belonging to different shells is small. Further, let us assume that we already have solved the secular equation in all subspaces $\mathcal{T}_n$ and found correct functions $\phi_\alpha^{(0)}$ in the zero approximation. Then in the first-order approximation the expansion coefficients of perturbed states i in the basis states α belonging to other shells will be [22]:

$$c_i^\alpha \cong \frac{\lambda V_{\alpha i}}{E_i^{(0)} - E_\alpha^{(0)}} \tag{21}$$

where $V_{\alpha i} = \langle \phi_\alpha^{(0)} | V | \phi_i^{(0)} \rangle$ and $E_\alpha^{(0)} = \epsilon_\alpha$ is the energy of states in a zero approximation (i.e. the unperturbed energy). The squared projection of a perturbed state ψ_i on the states belonging to the subspace orthogonal adjoint to $\mathcal{T}_N$ will be

$$\lambda^2 \sum_{\alpha \notin \mathcal{T}_N} \frac{|V_{\alpha i}|^2}{(E_i^{(0)} - E_\alpha^{(0)})^2}.$$

Now we should average this expression over all the $\dim \mathcal{T}_N$ states ψ_i (for small perturbations every state ψ_i can be approximately attributed to some $\mathcal{T}_n$):

$$W(\lambda, N) \cong \frac{\lambda^2}{\dim \mathcal{T}_N} \sum_{i \in \mathcal{T}_N} \sum_{\alpha \notin \mathcal{T}_N} \frac{|V_{\alpha i}|^2}{(E_i^{(0)} - E_\alpha^{(0)})^2}. \tag{22}$$

With increasing perturbation the parameter $W(\lambda, N)$ gradually grows (the basis states are fragmented over other shells) and at some critical value reaches 0.5. Thus a required critical perturbation parameter can be found from the equality

$$W(\lambda, N) = 0.5. \tag{23}$$

Let us prove now the invariance of $W(\lambda, N)$ with respect to arbitrary block unitary transformations $\hat{U}_b$ of the basis, which mixes the functions $\phi_\alpha^{(0)}$ only inside the irreducible representations $\mathcal{T}_n$ (i.e. inside one shell with the principal quantum number n). The functions from different shells are not mixed. It is possible to present the sum of the states $\alpha \notin \mathcal{T}_N$ as

$$\sum_{\alpha \notin \mathcal{T}_N} = \sum_{n \neq N} \sum_{\alpha \in \mathcal{T}_n}. \tag{24}$$

Therefore (22) can be written as

$$W(\lambda, N) = \frac{\lambda^2}{\dim \mathcal{T}_N} \sum_{n \neq N} W_n \tag{25}$$

$$W_n = \sum_{i \in \mathcal{T}_N} \sum_{\alpha \in \mathcal{T}_n} \frac{|V_{\alpha i}|^2}{(E_i^{(0)} - E_\alpha^{(0)})^2}. \tag{26}$$

Now consider what happens with the value W_n under the block unitary transformation $\hat{U}_b$ of the zero approximation basis wavefunctions

$$\phi_i^{(0)} \longmapsto \tilde{\phi}_i^{(0)} = \sum_\mu U_{\mu i} \phi_\mu^{(0)}. \tag{27}$$

Since the energies $E_i^{(0)}$ and $E_\alpha^{(0)}$ are the same for all states $i \in \mathcal{T}_N$ and $\alpha \in \mathcal{T}_n$ and do not vary under the transformation $\hat{U}_b$, the denominator in (26) can be taken out of the sum. Utilizing the symmetry in labels i and α it is sufficient to prove the invariance of W_n with respect to the unitary transformations of ϕ_i^0. Indeed,

$$\begin{aligned}
(E_i^{(0)} - E_\alpha^{(0)})^2 \tilde{W}_n &= \sum_{i \in \mathcal{T}_N} \sum_{\alpha \in \mathcal{T}_n} \langle \phi_\alpha^{(0)} | V | \tilde{\phi}_i^{(0)} \rangle \langle \tilde{\phi}_i^{(0)} | V | \phi_\alpha^{(0)} \rangle \\
&= \sum_{i \in \mathcal{T}_N} \sum_{\alpha \in \mathcal{T}_n} \langle \phi_\alpha^{(0)} | V \sum_\mu U_{\mu i} | \phi_\mu^{(0)} \rangle \sum_\nu U_{\nu i}^* \langle \phi_\nu^{(0)} | V | \phi_\alpha^{(0)} \rangle \\
&= \sum_\alpha \langle \phi_\alpha^{(0)} | V \sum_{\mu,\nu} \left(\sum_i U_{\mu i} U_{\nu i}^* \right) | \phi_\mu^{(0)} \rangle \langle \phi_\nu^{(0)} | V | \phi_\alpha^{(0)} \rangle \\
&= \sum_\alpha \langle \phi_\alpha^{(0)} | V \sum_\mu | \phi_\mu^{(0)} \rangle \langle \phi_\mu^{(0)} | V | \phi_\alpha^{(0)} \rangle \\
&= \sum_\alpha \sum_\mu |V_{\alpha\mu}|^2 = (E_i^{(0)} - E_\alpha^{(0)})^2 W_n.
\end{aligned}$$

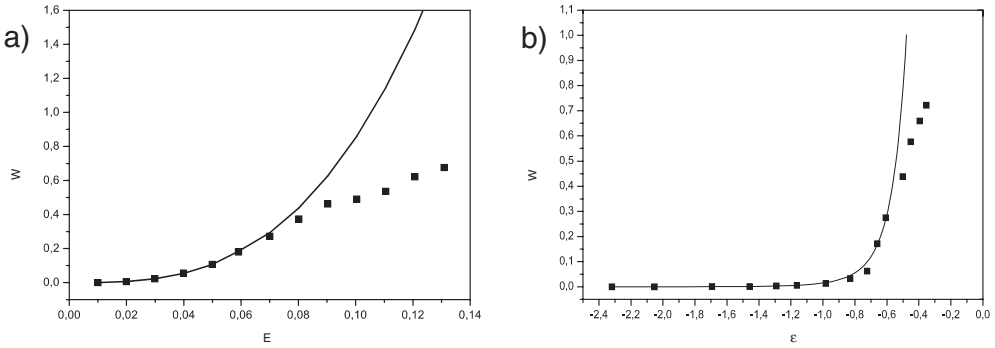

Figure 4. Perturbation theory (curve) and exact calculation (points) of the average squared projection W of wavefunctions on a subspace $\mathcal{H}\ominus\mathcal{T}_N$ as functions of energy in the (*a*) Henon–Heiles system and (*b*) for the diamagnetic Kepler problem.

Thus, making transformation $\hat{U}_b$ at first inside the subspaces $\mathcal{T}_N$, and then inside $\mathcal{T}_n$, we obtain the invariance of W_n with respect to $\hat{U}_b$. Since each term W_n in the sum (25) is invariant, all the sum $W(\lambda, N)$ will be also invariant with respect to unitary transformations.

This property allows us to bypass the necessity of solving the secular equation. We can use in the evaluation of $W(\lambda, N)$ in equation (22) the unperturbed basis functions ϕ_α and energy $E_\alpha^{(0)} = \epsilon_\alpha$ (2). Thus the obtained quantity $W(\lambda, N)$ may be used as an approximate measure of quantum chaoticity. It allows one to estimate the critical perturbation parameter value from the equality (23).

5. Tests of $W(\lambda, N)$ accuracy

In this section we shall compare the approximate estimates of the critical perturbation parameter with the exact calculations for a nonlinear Henon–Heiles Hamiltonian and diamagnetic Kepler problem. First we carried out exact 'head-on' calculations of $W(\lambda, N)$ using its definition (20). The spectra and eigenstates of the systems are calculated in the same manner as in section 3 (i.e. by the Hamiltonian matrix diagonalization). As an averaging range we selected the part of the spectrum, whose dim $\mathcal{T}_N$ eigenstates would have the maximal square of projection on the subspace $\mathcal{T}_N$. The results of these calculations are shown by the points on figure 4. Then we determined the approximate value of $W(\lambda, N)$ from equation (22) (curves in figure 4).

For the Henon–Heiles system (18) according to the exact calculation we achieve the critical value 0.5 at an energy $E_{cr} = 0.105$, which practically coincides with the above-obtained value $E_{cr} = 0.11$ according to the criterion æ $= 1$. As one should expect, the perturbation theory works well at small perturbation parameter (up to energies $E \approx 0.08$) and as a result yields the critical value of energy $E_{cr} = 0.084$.

The same test of the critical perturbation parameter estimate was carried out for the diamagnetic Kepler problem with Hamiltonian (19). Figure 4(*b*) shows the approximate values of $W(\lambda, N)$ (curve) and the exactly (see (20)) calculated ones (points) as functions of the scaled energy ϵ. As well as in the previous case, we have obtained the quite good agreement between the critical parameter value ($\epsilon_{cr} = -0.45$) obtained above (see section 3) with æ $= 1$ and as a result of exact calculations (20) and (23) ($\epsilon_{cr} = -0.47$). The approximate estimate (22) of $W(\lambda, N)$ coincides with the exact results up to $\epsilon \approx -0.6$ and gives the critical parameter value ($\epsilon_{cr} = -0.54$).

6. Conclusion

In this paper we continue to develop our approach to chaos in quantum stationary systems. Our main point is the connection between the symmetry properties of a system and its regularity or chaoticity. We confirmed that the previously suggested chaoticity measure $æ(\lambda, E)$ characterizes the initial symmetry breaking and destruction of the corresponding integrals of motion in a perturbed system, which leads to chaotization. Likewise in the case of the Henon–Heiles problem [7], the critical scaled energy value ϵ_{cr} when the parameter æ reaches unity corresponds to the onset of 'global' chaos on the classical phase portrait for the diamagnetic Kepler problem.

We also discussed the similarity of our criterion $æ = 1$ to the criterion of Hose and Taylor [21]. The coincidence of the critical parameters obtained with æ and exact W quantities confirms this similarity.

We have also suggested an approximate semi-analytical way to calculate $W(\lambda, N)$ in the framework of the perturbation theory. The approximate value of the critical perturbation parameter might be obtained from the relation (23) which contains matrix elements of perturbation V in the initial basis and energies of basis states. The comparison of this approximation with the exact results for the Henon–Heiles and the diamagnetic Kepler problems demonstrated that the accuracy of this approximation is about 10–20%.

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