The critical perturbation parameter estimate for the transition from regularity to chaos in quantum systems

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Abstract

In this paper we continue to develop our approach to the chaoticity properties of the quantum Hamiltonian systems. Our earlier suggested chaoticity criterion characterizes the initial symmetry breaking and the destruction of the corresponding integrals of motion in a perturbed system, which causes the system’s chaotisation. Transition from regularity to chaos in quantum systems occurs at a certain critical value of the perturbation parameter. In our previous papers we had to diagonalize the perturbed system’s Hamiltonian matrix in order to estimate this parameter. In the present paper we demonstrate that the critical perturbation parameter for the transition from regularity to chaos can be estimated in the framework of the first order perturbation theory. The values of thus obtained critical parameter are in good agreement with the results of our previous precise calculations for Hennon-Heiles Hamiltonian and diamagnetic Kepler problem.

1 Introduction

For last decades the investigations of quantum chaos have been extensively carried out but this field remains under hot discussions. One part of researchers believe that quantum chaos doesn’t exist and at best should be studied in the semiclassical approximation. It is believed that the quantum analogue of the classical system should have properties reflecting regularity or chaoticity of classical trajectories. The law of level spacing distribution is considered to be one of such properties. It is also believed that the quantum analogue of the classically chaotic system obeys Wigner level spacing law, while Poissonian law holds for regular systems. However many authors (including us [1]), pointed out the incompleteness and crudeness of this criterion of quantum chaoticity.

In this paper we continue to develop our approach [2-6] to the chaotic properties of the quantum Hamiltonian systems. Our main point is connection between the symmetry properties of a system and its regularity or chaoticity. We had demonstrated that our earlier suggested chaoticity parameter characterizes the initial symmetry breaking and destruction of the corresponding integrals of motion in a perturbed system, which leads to chaotisation. As it was shown in [3], in the semiclassical limit the chaoticity parameter transforms into

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Lyapunov’s exponent of the corresponding classical motion. We had also shown that according to our chaoticity criterion the transition from regularity to chaos in classical and quantum systems occurs at the same critical perturbation parameter.

In our previous papers we had to diagonalize the perturbed system’s Hamiltonian matrix in order to estimate this perturbation parameter. In this paper we shall show that it is possible to estimate it in the framework of the perturbation theory. In part 2 we reconsider the definition of our chaoticity parameter which is used for the investigation of the transition from regularity to chaos. Part 3 is devoted to the analytical estimate of the critical parameter in the framework of the first order perturbation theory. The comparison of our estimate with the precise calculations for Hennon-Heiles Hamiltonian and diamagnetic Kepler problem is done in part 4.

2 Destruction of quantum numbers and the chaoticity criterion

Consider a stationary quantum system with Hamiltonian $H$ as a sum of Hamiltonian $H_0$ of an integrable system and perturbation $\lambda V$, which destroys the symmetries of $H_0$ in such a way (see e.g. [3-4]) that the number $M$ of the independent first integrals of motion becomes less than the number of the system’s degrees of freedom:

$$H = H_0 + \lambda V.$$  \hspace{1cm} (1)

Eigenfunctions $\{\phi_\alpha\}$ of the unperturbed integrable Hamiltonian $H_0$ are common for some complete set of independent mutually commuting operators $\{J_\rho\}_{\rho=1}^N$ ($N$ - the number of degrees of freedom of the Hamiltonian $H_0$). Eigenstates $\psi_i$ of the full Hamiltonian may be expanded in eigenfunctions $\phi_\alpha$ of the unperturbed Hamiltonian $H_0$:

$$\psi_i = \sum_\alpha \phi_\alpha^* \psi_i \phi_\alpha = \sum_\alpha c_\alpha^i \phi_\alpha.$$  \hspace{1cm} (2)

Let us consider the probability $P_\alpha(E_i)$ to find the basis state $\phi_\alpha$ in the state $\psi_i$ with energy $E_i$, which is equal to the squared absolute value of the corresponding coefficient in (2) and define the energy width $\Gamma^\alpha_{spr}$ of $P_\alpha(E_i)$ distribution: the minimal energy interval for which the sum of probabilities $P_\alpha(E_i)$ is larger or equal to 0.5. Thus defined $\Gamma^\alpha_{spr}$ is the energy spreading width of basis state $\phi_\alpha$. The spectrum of $H_0$ may be degenerate and then the irreducible representations of the symmetry group of $H_0$ consist of several basis functions which belong to one energy level (shell). We want to find a parameter characterizing the measure of initial symmetry breaking of $H_0$ under the influence of the perturbation $V$. It’s clear that such symmetry breaking results only due to significant mixing between functions from different irreducible representations. The mixing of states within one shell doesn’t change their symmetry. While the spreading width $\Gamma^\alpha_{spr}$ is smaller then the distance $D_0$ between the neighboring levels in the spectrum of $H_0$ we can distinguish ”localization domain” (in energy) of one set of basis states from ”localization domain” of another one. When the spreading width exceeds $D_0$ we start loosing the ”traces” of basis functions in the spectrum of $H$ and can’t even approximately compare states $\psi_i$ with irreducible representation of symmetry group $H_0$. Thus a parameter

$$\alpha^\alpha = \Gamma^\alpha_{spr} / D_0$$  \hspace{1cm} (3)
is the natural measure of symmetry breaking. When the parameter $\alpha$ exceeds unity the symmetry of the Hamiltonian $H_0$ disappears. Such a value of perturbation is accompanied by disappearance of the initial selection rules, the levels are distributed approximately uniformly (level repulsion) and the level spacing distribution approaches Wigner’s law. One can say that the transition from regularity to chaoticity has taken place in quantum system and $\alpha$ may be considered as the parameter of chaoticity.

The spreading width $\Gamma_{spr}^\alpha$ depends on the number $\alpha$ of the basis state of Hamiltonian $H_0$, i.e. on its quantum numbers. The classical analogy to this is the dependence of the invariant torus stability on the corresponding values of integrals of motion. It is clear that in order to obtain the global chaoticity characteristic in quantum case it is necessary to average $\Gamma_{spr}^\alpha$ over the basis states $\phi_\alpha$ belonging to the same irreducible representation (shell). Thus we should determine the energy width $\Gamma_{spr}$ of the following distribution

$$P_N(E_i) = \frac{1}{\dim T_N} \sum_{\alpha \in T_N} |\phi_\alpha^* \psi_i|^2,$$

where $T_N$ is a degenerate level subspace with main quantum number $N$. The averaged parameter $\Gamma_{spr}$ unlike the local $\Gamma_{spr}^\alpha$ has an important feature of invariance with respect to the choice of the basis for the integrable Hamiltonian $H_0$ [1]. From the theoretical point of view the above chaoticity parameter has one more useful property. As it was shown in [3], in the semiclassical limit $\Gamma_{spr}^\alpha/\hbar$ transforms into Lyapunov’s exponent of the corresponding classical motion. Thus we see that parameter $\alpha(\lambda, E) = \Gamma_{spr}/D_0$ “measures” destruction (fragmentation) of the irreducible representations of the basis and, hence of the Casimir operator (the main quantum number), which is the approximate integral of motion for small perturbations.

## 3 Analytical estimate of the critical perturbation parameter

The analytical estimate can be performed in the following way: Firstly, the expansion coefficients (2) at small parameter $\lambda$ can be computed in the framework of usual perturbation theory. Secondly, since it is inconvenient to work with the distribution width $P_N(E_i)$ analytically, we shall use the equivalence of our chaoticity criterion based on $\alpha$ and the criterion of Hose-Taylor approach.

In a series of publications Hose and Taylor (see, e.g. [7,8]) in the framework of the theory of effective Hamiltonians 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 square projections of a perturbed wave function on model space is larger than 0.5. Operators commuting with effective hamiltonian will be approximate integrals of motions of the problem. Thus, if a square of a projection of some states $\psi_i$ of the Hamiltonian $H$ on space the $T_N$ of degenerate the level of $H_0$ are larger than 0.5, then the principal quantum number must be an approximate integral of motion for these states (in this range of energies). Therefore the average square of a projection of perturbed wave functions on subspace $T_N$ with fixed value of main quantum number should reach value 0.5 approximately at same critical perturbation when $\alpha = 1$ [5].

The principal problem in using the perturbation theory for estimating of squares of projections is the degeneracy of basis states and, hence, the necessity to solve a secular equation,
which prevents to obtain the analytical expressions. In order to bypass this complexity we shall act as follows. We shall construct such a quantity, which on the one hand will help us to estimate the critical perturbation parameter, and on the other will be invariant with respect to block unitary transformations inside subspaces $T_N$. This property will allow us in evaluating this quantity to utilize not only the states obtained from the secular equation, but also any others, generated from them by the block unitary transformations, (including the initial basis states $\phi_\alpha$). In this way we shall not need to solve the secular equation.

Let us estimate the average square of projection $W(\lambda, N)$ of the perturbed wave functions not on a subspace $T_N$, but on its orthogonal adjoint $H \ominus T_N$. Further, let us assume, that we already have solved the secular equation in all subspaces $T_N$ and found correct functions $\phi^{(0)}_\alpha$ in the zero approximation. Then in the first order approximation the expansion coefficients of perturbed states $i$ on basis $\alpha$ belonging to other shells will be:

$$c_{\alpha i} = \frac{V_{\alpha i}}{E_i(0) - E^{(0)}_\alpha},$$

where $V_{\alpha i} = \phi^{(0)}_\alpha \cdot V \phi^{(0)}_i$ and $E^{(0)}_\alpha$ is the energy of states in a zero approximation. The square of projection of a perturbed state $\psi_i$ on orthogonal adjoint to $T_N$ will be

$$\sum_{\alpha \notin T_N} \frac{|V_{\alpha i}|^2}{(E_i(0) - E^{(0)}_\alpha)^2}.$$ 

Now we average the previous expression over all $\text{dim} T_N$ states $\psi_i$ (for small perturbations every state $\psi_i$ can be approximately referred to some $T_N$):

$$W(\lambda, N) = \frac{1}{\text{dim} T_N} \sum_{i \in T_N} \sum_{\alpha \notin T_N} \frac{|V_{\alpha i}|^2}{(E_i(0) - E^{(0)}_\alpha)^2}. \quad (6)$$

With increasing perturbation the parameter $W(\lambda, N)$ will gradually grow (the basis states are fragmented over other shells) and at some critical value will reach 0.5. Thus a required critical perturbation parameter can be found by solving the equation

$$W(\lambda, N) = 0.5 \quad (7)$$

with respect to $\lambda$ or $N$.

Let us prove now the invariance of $W(\lambda, N)$ with respect to arbitrary block unitary transformations of the basis, which mixes the functions $\phi^{(0)}_\alpha$ only inside the irreducible representations $T_N$ (the functions from different $T_N$ are not mixed). It is possible to present the sum of the states $\alpha \notin T_N$ as

$$\sum_{\alpha \notin T_N} = \sum_{n \neq N} \sum_{\alpha \in T_n}. \quad (8)$$

Therefore (6) can be written as

$$W(\lambda, N) = \frac{1}{\text{dim} T_N} \sum_{n \neq N} W_n, \quad (9)$$

$$W_n = \sum_{i \in T_n} \sum_{\alpha \in T_n} \frac{|V_{\alpha i}|^2}{(E_i(0) - E^{(0)}_\alpha)^2}. \quad (10)$$
Now consider what happens with the value $W_n$ under the block unitary transformation $\hat{U}_b$ of the zero approximation basis wave functions

$$\phi_i^{(0)} \mapsto \tilde{\phi}_i^{(0)} = \sum_\mu U_{\mu i} \phi_\mu^{(0)}. \quad (11)$$

Since the energies $E_i^{(0)}$ and $E_\alpha^{(0)}$ are the same for all states $i \in T_N$ and $\alpha \in T_n$ and do not vary under the transformation $\hat{U}_b$, the denominator in (10) we can be taken out of the sum. Utilizing the symmetry in labels $i$ and $\alpha$ we can prove the invariance of $W_n$ with respect to their exchange. Indeed,

$$(E_i^{(0)} - E_\alpha^{(0)})^2 \tilde{W}_n = \sum_{i \in T_N} \sum_{\alpha \in T_n} (\phi_\alpha^{(0)} V \tilde{\phi}_i^{(0)})(\tilde{\phi}_i^{(0)} V \phi_\alpha^{(0)}) =$$

$$\sum_{i \in T_N} \sum_{\alpha \in T_n} \phi_\alpha^{(0)} V \sum_\mu U_{\mu i} \phi_\mu^{(0)} \sum_\nu U_{\nu i}^* (\phi_\nu^{(0)} V \phi_\alpha^{(0)}) = \sum_\alpha \phi_\alpha^{(0)} V \sum_\mu (\sum_i U_{\mu i} U_{\nu i}^*) \phi_\mu^{(0)} (\phi_\nu^{(0)} V \phi_\alpha^{(0)}) =$$

$$\sum_\alpha \phi_\alpha^{(0)} V \sum_\mu \phi_\mu^{(0)} (\phi_\mu^{(0)} V \phi_\alpha^{(0)}) = \sum_\alpha \sum_\mu |V_{\alpha \mu}|^2 = (E_i^{(0)} - E_\alpha^{(0)})^2 W_n.$$

Thus, making transformation $\hat{U}_b$ at first inside the subspaces $T_N$, and then inside $T_n$, we obtain the invariance of $W_n$ with respect to $\hat{U}_b$. Since each term $W_n$ in the sum (8) 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 to solve the secular equation. We can use in the evaluation of $W(\lambda, N)$ in Eq. (8) the initial basis functions $\phi_\alpha$ and energy $E_\alpha^{(0)}$, and find the critical perturbation parameter value from the equation (7).

\section*{4 Two examples}

In this part we shall compare the analytical estimates of the critical perturbation parameter with the precise calculations for a nonlinear Hennon-Heiles Hamiltonian and diamagnetic Kepler problem.

Let us consider a known Hennon-Heiles system with hamiltonian:

$$H(q, p) = \frac{1}{2}(p_1^2 + q_1^2) + \frac{1}{2}(p_2^2 + q_2^2) + \lambda(q_1^2 q_2 - q_2^3/3). \quad (12)$$

Introducing operators of creation and annihilation $a_k^\dagger = \frac{1}{\sqrt{2}}(q_k + ip_k)$, $a_k = \frac{1}{\sqrt{2}}(q_k - ip_k)$, $k = 1, 2$ we construct, as usual, the two-dimensional Cartesian oscillator basis

$$\phi_\mu = \phi_{n_1 n_2} = \frac{1}{\sqrt{n_1 n_2}} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \phi_0, \quad (13)$$

$$E_{n_1 n_2} = E_N = \hbar(n_1 + n_2 + 1).$$

It is easy to write out matrix elements of the Hamiltonian (12) in the basis (13) and to find through a diagonalization the system’s eigenvalues and eigenstates. In the calculations of bound states (with energies $E < 1/(6\lambda^2)$) the value $\lambda = 1$ and $\hbar = 0.01$ was fixed and the basis (13) was used, which included 496 of states (30 shells). We investigated average (over states with approximately equal energy) square of a projection of perturbed wave functions on subspace $\mathcal{H} \ominus T_N$. First we carried out precise calculations (see points on fig. 1), and then
Figure 1: Perturbation theory (line) and precise calculation (points) of average square of a projection of wave functions on a subspace $\mathcal{H} \ominus T_N$ dependence as functions of energy in the Hennon-Heiles system.

determined the value $W(\lambda, N)$ from Eq.(6) (line on Fig. 1). According to precise calculation we achieve critical value 0.5 at an energy $E \approx 0.105$, that practically coincides with earlier obtained [4] value with the criterion $\varepsilon = 1$ ($E \approx 0.11$). As one should to 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 $E \approx 0.084$.

The same test of the critical perturbation parameter estimate was carried out for diamagnetic Kepler problem with Hamiltonian

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

(14)

Here frequency $\omega = eB/2mc$, $B$ — magnetic field, directional along an axes $z$. Instead of the usual energy $E$ we used the standard dimensionless energy $\epsilon = E\gamma^{-2/3}$, where $\gamma = h\omega/R$ ($R$ — Rydberg constant). We diagonalized a matrix of the Hamiltonian in the Coulomb parabolical basis with quantum numbers $(n_1, n_2, m)$ and energies of basis states $E_n = -1/2n^2$; $n = n_1 + n_2 + |m| + 1$. For the investigation of a fragmentation of basis functions with $m = 0$ from a shell with the principal quantum number 10 we used the basis of the first 20 shells.

We studied the dependence of the average square of a projection of the perturbed wave functions on a subspace $\mathcal{H} \ominus T_N$ as a function of the scaled energy. As in the Hennon-Heiles case, we fixed a subspace $T_{10}$ with a main quantum number $N = 10$ and varied the values $\gamma$. As an averaging range we selected the part of the spectrum, whose states ($dimT_{10} = 10$) would have the maximum square of a projection on $T_{10}$. Fig. 2 shows the analytic result $W(\lambda, N)$ (line) and the numerically calculated (points) dependence of the precise wave functions’ average square projections on a subspace $\mathcal{H} \ominus T_{10}$ as functions of the scaled energy $\epsilon$. As well as in the previous case we have obtained the quite good agreement of the theoretical critical parameter estimate ($\epsilon_{cr} = -0.54$) with precise calculation ($\epsilon_{cr} = -0.47$), which is also in correspondence with earlier results [6] obtained using $\varepsilon = 1$ criterion ($\epsilon_{cr} = -0.45$).
Figure 2: Perturbation theory (line) and precise calculation (points) of average square of a projection of wave functions on a subspace $\mathcal{H} \ominus \mathcal{T}_{10}$ dependence as functions of scaled energy for a diamagnetic Kepler problem.

5 Conclusion

In this paper we continue to develop our approach [2-4] to the chaotic properties of the quantum Hamiltonian systems. Our main point is the connection between the symmetry properties of a system and its regularity or chaoticity. We show that the earlier suggested chaoticity parameter $\varepsilon(\lambda, E)$ characterizes the initial symmetry breaking and destruction of the corresponding integrals of motion in a perturbed system, which leads to chaotisation. The value of $\varepsilon$ is equal to the ratio of the average spreading width of the basis wavefunctions over the perturbed ones to the average unperturbed level spacings. In order to estimate the critical perturbation parameter for the transition from regularity to chaos we had to diagonalize the perturbed system’s Hamiltonian matrix. In the present paper we have shown that the critical perturbation parameter may be estimated in the framework of the first order perturbation theory. We construct a quantity which is invariant with respect to unitary transformations of subspaces $\mathcal{T}_N$ of basis degenerated levels $H_0$ and indicate the measure of system chaoticity. Thus there is no need to deal with secular equation and the approximate value of the critical perturbation parameter might be obtained from the relation which contains matrix elements of perturbation $V$ in the initial basis and energies of basis states. The values of thus obtained critical parameter are in good agreement with the results of our previous precise calculations for Hennon-Heiles Hamiltonian and diamagnetic Kepler problem.

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