Approximate integrals of motion and the quantum chaoticity problem
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Abstract

The problem of existence and constructing of integrals of motion in stationary quantum mechanics and its connection with quantum chaoticity is discussed. It is shown that the earlier suggested quantum chaoticity criterion characterizes destruction of initial symmetry of regular system and of basis quantum numbers under influence of perturbation. The convergent procedure allowing to construct approximate integrals of motion in the form of non-trivial combinations depending on operators \((q, p)\) is suggested. Properties of the obtained integrals with complicated structure and the consequences of their existence for system's dynamics are discussed. The method is used for explicit construction and investigation of the approximate integrals in Henon-Heiles 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 obvious from correspondence principle that quantum counterpart of 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 believed that the quantum analogue of the chaotic classical 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 [2-4] 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 show that the earlier suggested chaoticity criterion characterizes the initial symmetry breaking and destruction of the corresponding integrals of motion in a perturbed system, which leads to chaoticisation. We compare our approach with known criterion of existence of the approximate quantum numbers by Hose and Taylor [5, 6] which is based on the analysis of effective Hamiltonians.

One may ask if the new integrals of motion might appear in the perturbed system and how can they influence the system's dynamics. The problem of construction of the approximate integrals of motion has always attracted great attention due to its practical and philosophical importance. In classical mechanics we have KAM-theory which guarantees existence of invariant tori under perturbation; as to quantum mechanics the situation is somewhat tangled [5, 6]. The normal form method [7, 8] is well known for construction of the new approximate integrals of motion and integrable approximations to Hamiltonian. Its generalization on quantum systems was done in refs. [9-11]. After analyzing the reasons of divergence in the normal form method we propose a rather simple way for construction of approximate quantum numbers based on the unitary transformation of the basis integrals of motion.

In the final part of the paper we discuss the possibility of the exact integrals existence in the perturbed system and formulate the hypothesis of formal integrability in stationary quantum mechanics. We define formal integrability as the existence (in mathematical sense) of complete set of independent mutually commuting operators which have some characteristic
differences from the usual first integrals of motion. It is impossible to write such operators in closed form (they have extremely complicated structure) and we can’t find them before the solution of Schrödinger equation is obtained; these integrals don’t correspond to known symmetry groups and are non-separable. We discuss why such a formal (mathematical) integrability doesn’t contradict the system’s quantum chaoticity. The conception of chaos means that the system has algorithmic complexity (it is very difficult to solve equations with high accuracy) and statistical hypothesis works well in the system. The existence of non-separable integrals of motion with very complicated structure can’t help us to solve equations and doesn’t influence the validity of statistical hypothesis.

2 Destruction of quantum numbers and the chaoticity criterion

Presently we consider stationary quantum system with Hamiltonian \( H \) as a sum of Hamiltonian \( H_0 \) of an integrable system and perturbation \( \lambda V \): \[
H = H_0 + \lambda V. \tag{1}
\]

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 \( H_0 \): \[
\psi_i = \sum_{\alpha} \phi_{\alpha}^* \psi_i \phi_{\alpha} = \sum_{\alpha} c_{\alpha i} \phi_{\alpha}. \tag{2}
\]

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 \( \Gamma_{\text{spr}}^\alpha \) 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 \( \Gamma_{\text{spr}}^\alpha \) is the energy spreading width of basis state \( \phi_{\alpha} \). The spectrum of \( H_0 \) may be degenerate and then the irreducible representations of 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. Unless the spreading width \( \Gamma_{\text{spr}}^\alpha \) 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 ”signatures” 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 parameter \[
\alpha^\alpha = \Gamma_{\text{spr}}^\alpha / D_0 \tag{3}
\]
is the natural measure of symmetry breaking. When the parameter \( \alpha^\alpha \) 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 $\varphi^\alpha$ may be considered as the parameter of chaoticity.

The spreading width $\Gamma^\alpha_{spr}$ depends on the number $\alpha$ of 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 $\Gamma^\alpha_{spr}$ over the basis states $\psi_\alpha$ belonging to the same irreducible representation (shell). The averaged chaoticity parameter $\Gamma_{spr}$ unlike local $\Gamma^\alpha_{spr}$ has an important feature of invariance with respect to the choice of the basis for integrable Hamiltonian $H_0$ [12]. 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 $\Gamma^\alpha_{spr}/\hbar$ transforms into Lyapunov’s exponent of the corresponding classical motion.

Thus we see that criterion $\Gamma_{spr}$ ”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. The other quantum numbers of the basis states suffer destruction in general under a smaller perturbation due to the strong mixing within one shell. To define directly the degree of destruction of approximate integrals of motion one may use an ordinary mean-square-root deviation from the mean value. This deviation of some operator $A$ in the state $\psi_\alpha$ is calculated as follows:

$$
\Delta A = \sqrt{\psi_\alpha^*(A - \psi_\alpha^* A \psi_\alpha) \psi_\alpha}.
$$

(4)

The operator $A$ is the approximate integral of motion if the ratio of $\Delta A$ to the difference between its neighboring eigenvalues is less then 1.

Another way to study and construct the approximate integrals of motion is the well known method of effective Hamiltonians. In the series of works Hose and Taylor [5, 6] suggested the criterion of existence of the effective Hamiltonian and of connected with it integrals of motion. According to this criterion we may build the convergent sequence of approximations to the effective Hamiltonian under the condition that projection of perturbed Hamiltonian wave function to the model space is greater then 0.5. Thus if projection of some states $\psi_\alpha$ of Hamiltonian $H$ to the shell space exceeds $0.5$, then the main quantum number has to be the approximate integral of motion for these states. It is obvious that this criterion practically coincides with our spreading width one.

In order to compare the above criteria of destruction of the integrals of motion we have analysed the quantum Henon-Heiles system:

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

(5)

The eigenfunctions were obtained using the oscillator basis of 496 states (30 shells). Fig.1 shows the dependence on the perturbation intensity (energy $E$) of the parameter $\kappa$, the averaged spreading width of operator $N = n_x + n_y$ (see [1]) and of the averaged projection ($P_s$) of the exact wave functions to the shell. For the sake of easier comparison with other quantities in Fig.1 we plotted the value $Pr = 2(1 - P_s)$. We see that destruction of the initial $SU(2)$-symmetry according to all these three criteria takes place approximately at $E = 0.10$.

Thus $\Gamma_{spr}$ measures the degree of mixing between the irreducible representations and the destruction of the corresponding Cazimir operators. The question arises if some new integrals of motion might appear instead of the destroyed basis integrals.
The method of normal forms is the most known way to construct the approximate integrals and the integrable approximations to Hamiltonian in classical mechanics \cite{7, 8}. It has been generalized on quantum systems in refs. \cite{9-11}. In this method the perturbed wave functions are constructed as certain superposition of the basis functions belonging to a single irreducible representation. Therefore the symmetry of the wave functions is not changed and perturbation $V$ with lower symmetry leads only to the splitting of the degenerated level.

This approach gives rather good results when the perturbation is small. However Siegel (1941) proved the divergence of classical normal forms in the case of nonintegrable initial system. In quantum mechanics the question about convergence hasn’t got a final solution, though the authors \cite{10, 11} stress the asymptotic character of the series arising and confirm it by numerical calculations.

Two reasons for the divergence in the method of normal forms may be pointed out. The first one is well known — it is the non-analyticity of solutions at the point $\lambda = 0$ (the replacement $\lambda \to -\lambda$ in Hamiltonian may lead to significant changes of spectrum properties) and, as a consequence, to the divergence of the expansion into the powers of $\lambda$. The second reason is as follows. In the quantum Birkhoff-Gustavson method the integrable approximations are constructed in the form of power series of operators which mix basis states only inside one irreducible representation of the basis symmetry group (one shell). If the interaction effectively mixes states from different irreducible representations the Birkhoff-Gustavson method obviously can’t generate good integrable approximations and convergent integrals in principle. This is why the quantum numbers given by normal form might be good only when mixing between the different shells is weak ($\Gamma_{spr} < 1$).

The difficulties described doesn’t mean the principal absence of approximate integrals of motion in the perturbed system, they only reveal the shortcomings of the methods. To get a convergent method of constructing the integrals one should use combinations of operators which mix states in any given finite-dimensional subspace. In this case we can improve the integrable approximation to $H$ (in the sense of operator norm) by simply increasing the dimensions of this subspace. In the next section we’ll describe the convergent procedure allowing to construct approximate integrals in a rather trivial way.

### 3 The convergent method for integrals of motion

Performing a unitary transformation $U$ of some basis with a set of quantum numbers we can always easily find a new set of mutually commuting operators for which a transformed basis functions are eigenfunctions. One can see that $J'_\rho = U J_\rho U^\dagger$ ($J_\rho$ — operators of initial basis) are the desirable operators and such bases are equivalent in the sense of the quantity of quantum numbers. If we assume the completeness of eigenstates $\psi_\alpha$ of Hamiltonian $H$ in the Hilbert space $\mathcal{H}$ then $\psi_\alpha = U \phi_\alpha$ ($\phi_\alpha$ is the eigenfunction of $H_0$), because any two complete orthonormal bases are connected via some unitary transformation $U$. Operators $J'_\rho$ commute with $H$ in the full Hilbert space $\mathcal{H}$. Actually, for any function from complete basis $\psi_\alpha$

$$[H, J'_\rho] \psi_\alpha = HU J_\rho U^\dagger \psi_\alpha - U J_\rho U^\dagger H \psi_\alpha = HU J_\rho \phi_\alpha - E_\alpha U J_\rho \phi_\alpha =$$

$$j_{\rho \alpha} H U \phi_\alpha - E_\alpha j_{\rho \alpha} U \phi_\alpha = j_{\rho \alpha} E_\alpha \psi_\alpha - E_\alpha j_{\rho \alpha} \psi_\alpha = 0.$$

$J'_\rho$ are derived from $J_\rho$ with the aid of unitary transformation, hence they also form a complete set of independent commuting operators and their eigenvalues $j_{\rho \alpha}$ uniquely define every eigenstate $\psi_\alpha$ of Hamiltonian $H$. Therefore $H$ is a function depending on operators
\( J'_\rho \): \( H = H(J'_\rho) \), and \( E_\alpha = H(j_{\rho\alpha}) \). Having determined the approximate wave functions of perturbed Hamiltonian we can construct the unitary transformation \( U \) and the approximate integrals of motion \( J'_\rho \). The question about convergence of the procedure suggested is reduced to investigating whether the corresponding method for solving of Schrödinger equation converges or not. For example it has been proved that Ritz’s method converges (with increasing basis) in the case of Hermitian operators with lower-bounded discrete spectrum [13].

The introduced operators \( J'_\rho \) seem to be formal unless we construct them explicitly as functions of dynamic variables \((q, p)\). This, however is not difficult to do with the help of methods taken from the theory of continuous groups’ representations. In the remaining part of this section the realization of this method is described in details and properties of the integrals obtained are discussed.

Let us consider Schrödinger equation \( H\psi = E\psi \) with discrete spectrum \( E_\alpha \) and \( \psi_\alpha \) and write the Hamiltonian \( H \) in the form of spectral decomposition

\[
H = \sum_{\alpha} E_\alpha \psi_\alpha \psi^*_\alpha.
\]  

(6)

We represent the complete Hilbert space \( \mathcal{H} \) as a sum of the finite-dimensional model space \( \mathcal{P} \) and its orthogonal adjunct \( \mathcal{Q}: \mathcal{H} = \mathcal{P} + \mathcal{Q} \). It is convenient to construct the space \( \mathcal{P} \) of eigenfunctions \( \{\phi_\mu\}_{\mu=1}^{\text{dim}\mathcal{P}} \) by using some complete set of mutually commuting operators \( \{J_\rho\}_{\rho=1}^{N} \) \((N - \text{the number of degrees of freedom } H)\). We’ll find the approximate wave functions of \( H \) in the \( \mathcal{P} \)-space as a combination of basis states \( \phi_\mu \) (as, for example, in Ritz’s variational method or in different versions of perturbation theory)

\[
\psi_{\rho\alpha} = \sum_{\mu \in \mathcal{P}} c_{\alpha}^\rho \phi_\mu.
\]  

(7)

Orthonormal states \( \psi_{\rho\alpha} \) are derived from minimum condition for the energy functional in the \( \mathcal{P} \)-space and they form a subspace in the \( \mathcal{P} \)-space (obviously, only a small number of combinations \( \{\phi_\mu\} \) will satisfy Schrödinger equation with sufficient accuracy). We’ll denote this subspace of solutions by \( \mathcal{S} \) and the energy of states by \( E_{\rho\alpha} \). The rest \( \text{dim}\mathcal{P} - \text{dim}\mathcal{S} \) of the basis functions in the \( \mathcal{P} \)-space may be chosen arbitrarily, and we denote the new basis in the \( \mathcal{P} \)-space \( \{\phi'_{\mu}\}_{\mu=1}^{\text{dim}\mathcal{P}} \) (\( \phi'_{\mu} = \psi_{\rho\mu}, \mu = 1, ..., \text{dim}\mathcal{S} \)). Let us show that the operator

\[
H_s = \sum_{\alpha \in \mathcal{S}} E_{\rho\alpha} \psi_{\rho\alpha} \psi^*_{\rho\alpha}
\]  

(8)

(i) commutes with operators forming a complete set in the full Hilbert space \( \mathcal{H} \), i.e. it is integrable, (ii) \( H_s \) is approximating \( H \) in the sense of operator norm in the \( \mathcal{S} \)-space, (iii) \( H_s \) may be expressed in terms of dynamic variables \((q, p)\) as well as the initial Hamiltonian \( H \).

By calculation of wave functions \( \psi_{\rho\alpha} \) we constructed simultaneously the unitary transformation \( \phi'_{\mu} = U \phi_\mu \) of space \( \mathcal{H} \), which is defined by coefficients \( c_{\alpha}^\rho \) in the \( \mathcal{P} \)-space and is the identical transformation in the \( \mathcal{Q} \)-space. Operators \( J'_\rho = U J_\rho U^\dagger \) are known to form the complete set with the same quantum numbers \( j_{\rho\alpha} \) and eigenfunctions \( \phi'_{\mu} \). As far as eigenfunctions of operators \( J'_\rho \) and \( H_s \) in the \( \mathcal{S} \)-space coincide, the operators commute in this space. Outside the \( \mathcal{S} \)-space \( H_s \equiv 0 \) and hence it also commute with \( J'_\rho \). Therefore \([H_s, J'_\rho] = 0\) in the full space \( \mathcal{H} \).

Now we are going to check that Hamiltonian \( H_s \) is close to \( H \) in the sense of the operator norm in \( \mathcal{H} \), i.e. \( \|H - H_s\|_S < \epsilon \), under the condition that the residual of the approximate
solutions \((H - E_{\rho\alpha})\psi_{\rho\alpha} = \delta\psi_{\alpha}\) doesn’t exceed \(\epsilon\): \(\|\delta\psi_{\alpha}\| < \epsilon\). Really, for an arbitrary function \(\chi = \sum a^\delta\psi_{\delta}\), \(\|\chi\| = 1, \chi \in {\mathcal S}\)

\[
\|H\chi - H_s\chi\| = \|((\sum_{\alpha \in {\mathcal H}} E_{\alpha}\psi_{\alpha}\psi_{\alpha}^* - \sum_{\alpha \in {\mathcal S}} E_{\rho\alpha}\psi_{\rho\alpha}\psi_{\rho\alpha}^*) \sum_{\delta \in {\mathcal S}} a^\delta\psi_{\delta})\| =
\]

\[
\|\sum_{\delta \in {\mathcal S}} a^\delta(\sum_{\alpha \in {\mathcal H}} E_{\alpha}\psi_{\alpha}\psi_{\alpha}^* - E_{\rho\delta}\psi_{\rho\delta})\| \leq \epsilon \sum_{\delta \in {\mathcal S}} |a^\delta| \leq \epsilon \sqrt{\dim{\mathcal S}}.
\]

In the last estimate we used the fact that \(\sum |a^\delta|\) under the condition \(\sum |a^\delta|^2 = 1\) reaches its maximum value when all \(a^\delta\) are identical and equal to \(1/\sqrt{\dim{\mathcal S}}\). The accuracy \(\epsilon\) depends on dimensionality of \({\mathcal P}\)-space; we may fix \(\dim{\mathcal S}\) and decrease \(\epsilon\) in such way that the norm \(\|H - H_s\|\) should be as small as we need.

The introduced operators \(H_s\), \(U\) and \(J'_\mu\) seem to be formal unless we construct them explicitly as functions of dynamic variables \((q, p)\). Writing operator \(\psi_{\rho\alpha}\psi_{\rho\alpha}^*\) in terms of expansion (7) we have:

\[
H_s = \sum_{\mu, \nu \in {\mathcal P}} \left\{ \sum_{\alpha \in {\mathcal S}} E_{\rho\alpha} c^\alpha c_{\nu}^\alpha \right\} \phi_\mu \phi_\nu^*.
\]

The operator \(U\) may be also represented as a combination of basis operators \(\phi_\mu \phi_\nu^*\):

\[
U = 1 + \sum_{\alpha \neq \beta \in {\mathcal P}} U_{\alpha\beta} \phi_\beta \phi_\alpha^* + \sum_{\gamma \in {\mathcal P}} (U_{\gamma\gamma} - 1) \phi_\gamma \phi_\gamma^*.
\]

The first \(\dim{\mathcal S}\) rows of the unitary matrix \(U_{\alpha\beta}\) coincide with matrix \(c^\beta\), the rest \(\dim{\mathcal P} - \dim{\mathcal S}\) may be chosen in arbitrary way. It is easy to verify that components \(\chi\) don’t change outside \({\mathcal P}\) when \(U\) acts on arbitrary state \(\chi = \sum a^\delta\phi_\delta\), while inside \({\mathcal P}\) they are transformed by unitary matrix:

\[
U\chi = \sum_{\delta \in {\mathcal P}} a^\delta\phi_\delta + \sum_{\alpha \in {\mathcal S}} \left( \sum_{\beta \in {\mathcal P}} U_{\beta\alpha} a^\beta \right) \phi_\alpha.
\]

Now we’ll construct the basis operators \(\phi_\mu \phi_\nu^*\) as ordinary operators in the form of combinations depending on variables \((q, p)\) and acting on states of Hilbert space in co-ordinate representation. If \(G\) is the group of transformations corresponding to the complete operator set \(J_{\mu}(q, p)\), then \({\mathcal P}\)-space is in general a direct sum of irreducible representations \(T_s\) of the group \(G\):

\[
{\mathcal P} = \sum_s \oplus T_s.
\]

Operator \(\phi_\mu \phi_\nu^*\) transforms the function \(\phi_\nu\) into \(\phi_\mu\). If the group \(G\) is Abelian one, the irreducible representations \(T_s\) are one-dimensional and consist of the function \(\phi_s\). For non-Abelian group \(\phi_\mu\) and \(\phi_\nu\) may belong to one irreducible representation. Our aim is to write the operators which generate all possible transitions between different \(T_s\) and within some \(T_s\) as well. It’s not difficult to solve this problem by methods of group theory and actually the problem is equivalent to the realization of the basis \(\phi_\mu\).

To perform transformations inside the irreducible representations \(T_s\) it’s sufficient to use combinations of generators of the basis symmetry group; to connect different \(T_s\) we need generators of special non-invariance group of basis. Its infinite-dimensional irreducible representation is spanned on our basis. We know non-invariance groups and corresponding algebras for various bases, for example, \(so(4, 2)\) — for Coulomb’s basis and \(so(3, 2)\) — for isotropic two-dimensional oscillator basis [14]. After realization of operators of non-invariance algebra \(A_{\alpha}\) in the form of combinations of dynamic variables \((q, p)\) we look for vacuum state \(\phi_0\) for
which the decreasing operators from the set $A_\alpha(q,p)$ give zero. The vacuum state forms one-dimensional irreducible representation of symmetry group $\mathcal{G}$, and we shall naturally obtain states from other irreducible representations $\mathcal{G}$ acting on it with creation operators from the set $A_\alpha$. Notation $S^\dagger_\mu(A_\alpha)$ defines the operator composed of generators $A_\alpha$ which produces basis function $\phi_\mu$: $\phi_\mu = S^\dagger_\mu \phi_0$. We don’t present the general formula for $S^\dagger_\mu = S^\dagger_\mu(A_\alpha)$ because it is not difficult to do it in any specific case (see section 4); usually $S^\dagger_\mu$ are polynomials composed of generators $A_\alpha$ the power of which increases with state’s number $\mu$. Then operator $\phi_\mu \phi^*_\nu$ on the Hilbert space $\mathcal{H}$ may be written as follows:

$$\phi_\mu \phi^*_\nu = S^\dagger_\mu S_\nu P_\nu,$$

where $P_\nu$ is the projector on the state $\phi_\nu$. The projector $P_\nu$ may also be expressed in terms of dynamic variables $(q,p)$ in the following way. Let $T(x)$ be the operators of unitary representation $\mathcal{G}$ in Hilbert space, $D^*_{\alpha_\beta}(x)$ — matrix elements of irreducible representation $\mathcal{T}_\alpha$, $dx$ — invariant Haar’s measure on $\mathcal{G}$. Then the projector $P_\nu$ on the basis state $\phi_\nu \in \mathcal{T}_\alpha$ may be presented as [15]:

$$P_\nu = \dim \mathcal{T}_\alpha \int_G dx D^*_{\nu\nu}(x)T(x).$$

Operators [12] are bounded, and since $T(x)$ is the exponent to the power of generators $\mathcal{G}$ which form sub-algebra with respect to operator algebra $A_\alpha(q,p)$, we have achieved our goal — expressed the basis operators $\phi_\mu \phi^*_\nu$, $H_\delta$ (9), $U$ (11) and integrals $J^\rho$, in terms of variables $(q,p)$.

Thus constructed integrable approximations $H_\delta(q,p)$ and integrals of motion $J^\rho(q,p)$, apart from their approximate character (the commutators with $H$ are not exactly equal to zero) are local. The Hamiltonian $H_\delta$ is close to $H$ in the sense of operator norm only in the finite-dimensional subspace $S$, while the operators $J^\rho$ are good invariants also only in the $S$-space (outside the $P$-space they coincide with the old operators $J^\rho$). In the following section we shall demonstrate how the method works in Henon-Heiles problem and then continue to discuss the properties of the integrals obtained.

### 4 Approximate integrals in Henon-Heiles problem

Here we apply the method of the integral construction developed in the previous sections to the well known Henon-Heiles problem with Hamiltonian (5). Introducing operators of creation and annihilation $a^\dagger_k = \frac{1}{\sqrt{2}}(q_k + ip_k), a_k = \frac{1}{\sqrt{2}}(q_k - ip_k), k = 1, 2$ we construct, as usual, the Cartesian oscillator basis

$$\phi_\mu = \phi_{n_1 n_2} = \frac{1}{\sqrt{n_1! n_2!}}(a^\dagger_1)^{n_1}(a^\dagger_2)^{n_2} \phi_0$$

We present the projector $P_{n_1 n_2}$ on the state $\phi_{n_1 n_2}(q_1, q_2) = \phi_{n_1}(q_1) \otimes \phi_{n_2}(q_2)$ as a product of projectors on the states $\phi_{n_1}(q_1)$ and $\phi_{n_2}(q_2)$ of the corresponding one-dimensional oscillator. For one-dimensional oscillator $\mathcal{G} = U(1)$, $T(x) = e^{ia^1ax}$, $x \in [0, 2\pi]$, $D^*_{\nu\nu} = e^{i\nu x}$, where the number of state $\nu$ equals the number of quanta in this state. Then according to (12)

$$P_n = \int_0^{2\pi} \frac{dx}{2\pi} e^{-i\nu x} e^{ia^1ax} = -\frac{i}{2\pi}(a^\dagger a - n)^{-1}\{e^{2\pi i(a^1a - n)} - 1\} =$$

$$\frac{1}{\pi}(a^\dagger a - n)^{-1}e^{\pi i(a^1a - n)} \sin \pi(a^\dagger a - n) = \frac{1}{\pi}(a^\dagger a - n)^{-1} \sin \pi(a^\dagger a - n).$$
We neglect the phase in the last expression because it does not affect the action of \( P_n \). It’s easy to check that \( P_n \) acts in the necessary way due to its slightly exotic form:

\[
P_n \phi_\mu = \delta_{n\mu} \phi_\mu.
\]

The total projector \( P_{n_1 n_2} \) takes the form

\[
P_{n_1 n_2} = \frac{1}{\pi^2} (a_1 \dagger a_1 - n_1)^{-1} (a_2 \dagger a_2 - n_2)^{-1} \sin \pi (a_1 \dagger a_1 - n_1) \sin \pi (a_2 \dagger a_2 - n_2). \tag{14}
\]

As a result the formulae (13) together with (13) gives us the operator \( \phi_\mu \phi_\nu^* \):

\[
\phi_\mu \phi_\nu^* = \frac{(a_1 \dagger)^{n_1(\mu)} (a_2 \dagger)^{n_2(\mu)} (a_1)^{n_1(\nu)} (a_2)^{n_2(\nu)}}{\sqrt{n_1(\mu)! n_2(\mu)!} \sqrt{n_1(\nu)! n_2(\nu)!}} P_{n_1(\mu) n_2(\nu)}, \tag{15}
\]

where \( n_1 \) and \( n_2 \) are the quantum numbers of states. Using (8), (14) and determining coefficients \( c_\alpha^\mu \) and \( E_{p\alpha} \) we get integrable approximation \( H_s \) and approximate integrals \( J'_\rho = U J_\rho U^\dagger \). We may take \( n_1 \) and \( n_2 \) or \( n_1 \) and \( n = n_1 + n_2 \) as independent integrals \( J_\rho (\rho = 1, 2) \). The coefficients of expansion \( c_\alpha^\mu \) and the energies \( E_{p\alpha} \) were calculated by Ritz’s method with the aid of diagonalization of matrix \( H \) on the basis (13). We shan’t write explicit expressions for \( J'_\rho \) for they are very cumbersome: if \( D \) is the basis dimensionality, then operators \( J'_\rho \) consist of \( D^4 \) terms of the type (15). To determine the degree of destruction of approximate integrals of motion \( J'_\rho \) in the states \( \psi_\alpha \), we calculate the mean-square-root deviation \( J'_\rho \) with the help of (13). The solutions obtained with the basis of 496 states (30 shells) were considered to be true wave functions. Fig.2 shows the dependence of averaged measure of destruction (13) of operators \( J'_\rho (J_1 = l \ J_2 = n) \) on the perturbation intensity (energy \( E \)) in the subspaces with different symmetries. Henon-Heiles Hamiltonian has a symmetry \( C_{3v} \). Therefore the eigenfunctions’ space can be divided into 4 subspaces \( A, B, C, D \) (the states belonging to \( C \) and \( D \) subspaces have the same energy and thus produce the sequences of degenerate levels). The approximate integrals \( J'_\rho \) were calculated for the \( P \)-space of different dimensionalities (1, 10, 15 and 20 shells). One can see that increasing of \( P \)-space dimensionality is accompanied by the decrease of fragmentation of the approximate integrals in the \( S \)-space; outside the \( S \)-space operators \( J'_\rho \) loose their advantages in comparison with \( J_\rho \).

This example shows that the approximate integrals \( J'_\rho \) really have smaller spreading (fragmentation) in the \( S \)-space then the basis integrals of motion \( J_\rho \). We may get very small values \( \Delta J'_\rho \approx 0 \) for the bounded states by increasing of \( dim P \). As a result the analytical structure of \( J'_\rho \) becomes very complicated.

5 Are integrability and chaos compatible?

Now we consider the question about the convergence of the suggested procedure and the question about existence of exact integrals of motion of Hamiltonian \( H \) in the full Hilbert space (integrability of \( H \)). With the help of Ritz’s method we can find in principle any finite number of states with any finite accuracy and thus construct integrable approximation \( H_s \) to \( H \) and integrals \( J'_\rho \) in any finite subspace with any desirable accuracy. The question is: can we obtain the full infinite spectrum of \( H \) by tending \( P \to H \), because there is an effect of systematic ”delay” of \( S \)-space dimensionality with respect to dimensionality of the model \( P \)-space (only states far from the boundary of the approximate spectrum are
reasonably accurate in diagonalization). In other words, does the sequence of Hamiltonians $PHP$ converge to the initial Hamiltonian: $PHP \rightarrow H$ while $P \rightarrow 1$. Physically it seems to be so but we are in a difficulty to give rigorous mathematical proof, because the sequence $PHP$ is not Caushy’s sequence in the sense of operator norm in $\mathcal{H}$.

We can formulate the following hypothesis about integrability of $H$. If there exist a good (in mathematical sense) unitary operator $U$ connecting two complete orthonormal bases: the initial $\phi_\alpha$ and the basis of eigenstates $\psi_\alpha$, then the Hamiltonian $H$, as we have seen above, commutes with the complete set of independent operators $J^\rho_\alpha$ and it may be expressed in terms of only these variables $H = H(J^\rho_\alpha)$. (Moreover, according to Dirac [16] any functions of arbitrary complete orthonormal basis are eigenfunctions of some complete set of commuting observables. This allows to extend our conclusions for any observable, including the case of continuum spectra). Therefore the Hamiltonian $H$ seems to be formally integrable. However, in the above considered example (the Henon-Heiles Hamiltonian) the system is chaotic according to all the criteria of Section 2. Moreover, we know for sure that in the classical limit this system is one of the textbook examples of chaoticity. The problem is how to remove the contradiction between the seeming formal integrability and the chaoticity of the system.

One possible answer is connected with the properties of the new integrals $J^\rho_\alpha$. These integrals of motion are independent and global (provided the convergence of $PHP$ discussed above would be proved). However they have extremely complicated structure and can’t be expressed in closed form. Therefore they are useless to separate variables (non-separable) and to solve a problem. We restore them after the approximate numerical solution has been found. These integrals don’t give selection rules for transitions between levels. Therefore they are definitely not the quantum analogs of the classical first (isolating) integrals, which define the classical regular integrable system.

6 Conclusions

The problem of existing and constructing of integrals of motion in stationary quantum mechanics and its connection with notion of quantum chaoticity has been investigated. It has been shown that the previously suggested quantum chaoticity criterion characterises destruction of initial symmetry of regular system and basis integrals of motion under the influence of perturbation. Our approach conforms with known probability criterion of Hose and Taylor [5-6] and direct estimate of fragmentation (4).

We use variational Ritz’s method for explicit construction of approximate integrals of motion in the form of combinations depending on operators $(q, p)$ though in principle another method for solving Schrödinger equation may be used. As a result we obtained finite large-dimensional sums consisting of non-invariance algebra operators in various powers and projectors nontrivially expressed in terms of invariance algebra generators. The quality of approximate integrals of motion is simply controlled by dimensionality of model space in use.

These integrals of motion are independent and global (provided the convergence of $PHP \rightarrow H$ discussed above would be proved). However they have extremely complicated structure but have extremely complicated structure and can’t be expressed in closed form, therefore they are useless to separate variables (non-separable). This also explains why the existence of these integrals doesn’t create obstacles to statistical description of quantum
system. That’s why such formal integrability (even if we’ll prove the existence of global integrals rigorously) doesn’t make system to be regular in the sense of absence of chaotic properties. Therefore they are definitely not the quantum analogs of the classical first (isolating) integrals, which define the classical regular integrable system.

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Fig. 2