Abstract

The statistics of quantum Poincaré recurrences in Hilbert space for diamagnetic hydrogen atom in strong magnetic field has been investigated. It has been shown that quantities characterizing classical chaos are in a good agreement with the ones that are used to describe quantum chaos. The equality of classical and quantum Poincaré recurrences has been shown. It has been proved that one of the signs of the emergence of quantum chaos is the irreversible transition from a pure quantum mechanical state to the mixed one.

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1 Introduction

The investigation of the chaotic processes in the deterministic systems is one of the most important trends of the modern physics [1–5]. The successes of this current for nonlinear classical systems that are described via trajectories of the system in Hilbert space are obvious [6–8]. Yet the conception of deterministic chaos in quantum systems, where the idea of trajectory is inapplicable, stays a subject for serious discussions so far. There is no common understanding of the problem of quantum chaos for today. Usually the quantum chaos is considered as a set of phenomena taking place in quantum systems, the classical analogues of which display chaos [9–16].

Generally when investigating the problems of quantum chaos, one has to deal with the Hamiltonians of the form:

\[
\hat{H}(p, q, \lambda) = \hat{H}_0(p, q) + \lambda V(q),
\]

(1.1)

where p, q are a set of classical coordinates and momentum, \(\hat{H}_0(p, q)\) is classically integrable part of Hamiltonian, \(V(q)\) is a part of Hamiltonian which leads to the nonintegrability of the classical equations of motion when added, \(\lambda\) is a parameter by variation of which the system may be driven in the domain of chaotic dynamics.
The goal of this work is the investigation of a concrete physical system described by the Hamiltonian of the form (1.1). The object of our investigation is a diamagnetic hydrogen atom placed in a strong magnetic field. Diamagnetic hydrogen atom, subjected to the influence of the strong magnetic field, has been considered in the quasi-classical approximation in the ref [16]. Namely a photo-absorption spectrum in the transition regime to chaos has been studied. The main purpose of our work is the investigation of the irreversible evolution of the quantum-mechanical system and the passage from the quantum-mechanical to the quantum-statistical consideration. We shall try to compare and find out the link between the phenomena taking place under both classical and quantum considerations.

Relatively weak magnetic field applied to atom leads just to the energy levels splitting, i.e. to the Zeeman effect. In case when the hydrogen atom is placed in the extreme high magnetic field, the motion of the electron in the plane perpendicular to the field direction is completely defined by this magnetic field and not by the coulomb field of the nucleus, and because of this, the atom is found to be deformed in the transverse direction. At the same time the field does not affect on the lengthwise motion, and in this direction the atom keeps its size.

One may easily estimate the value of the magnetizing force when the deformation of the electron shell takes place. One has to compare the value of Bohr radius \(a_0 = \hbar^2/m_e e^2\) (where \(\hbar\) is a Plank constant, \(m_e\) and \(e\) are the electron mass and charge respectively) with a characteristic size of the localization domain of electrons in the magnetic field in the ground state when \(n = 0, s = 0\), \(a_B = \sqrt{\hbar c/eB}\). If \(a_B < a_0\), then the magnetic field has the defining effect. This condition leads to the following estimate of the extremely strong field

\[
B > \frac{m_e^2 c e^3}{\hbar^3} = B_c = 2.35 \cdot 10^5 T s,
\]

in which the atom is deformed. Notice, that the magnetic fields required for this, the intensity of which is defined by the condition (1.2), according to the modern concepts, may exist on the surface of some astrophysical objects. The neutron stars (or pulsars) appearing as the result of the collapse of the supernova, belong to them. That is why the investigation of the diamagnetic atoms in the conditions of extremely high magnetic fields is of doubtless interest.

2 Classical Consideration

Consider the hydrogen atom placed in the magnetic field directed along z-axis \(\vec{B} = B\vec{e}_z\). We shall use Larmor theorem. According to this theorem, for studying the diamagnetism theory for single atoms it is enough to consider the motion of the electron in the coordinate system, rotating with the Larmor frequency \(\omega_L = \gamma_c \vec{B}\), where \(\gamma_c\) is a gyromagnetic ratio for electrons.

During the transition to the rotating coordinate system, the change of the kinetic energy of the electron will occur. This change is conditioned by the
addition to the velocity of in the rotating coordinate frame \( \vec{u} \) the cross-product of the Larmor frequency \( \vec{\omega}_L \) and the vector \( \vec{r} \) of the location of electron. Taking into account, that the direction of vector \( \vec{\omega}_L \) is opposite to the vector \( \gamma_e \vec{B} \), and gyromagnetic ratio of the electron is \( \gamma_e = -\frac{e}{2m_e c} \) (here \( c \) is the velocity of light), we shall achieve for the velocity of electron in a motionless coordinate frame:

\[
\vec{v} = \vec{u} + [\vec{\omega}_L \vec{r}] = \vec{u} + \frac{e}{2m_e c} [\vec{B} \vec{r}].
\]

Then the kinetic energy of the electron will be of form:

\[
K = \frac{1}{2} m_e u^2 + m_e [\vec{\omega}_L \vec{r}] \vec{u} + \frac{1}{2} m_e |[\vec{\omega}_L \vec{r}]|^2 =
\]

\[
= \frac{1}{2} m_e u^2 + \frac{e}{2m_e c} B L_z + \frac{e^2}{8m_e c^2} B^2 (x^2 + y^2).
\]

One may easily see, that if z-projection of the angular momentum is equal to zero, \( L_z = 0 \) the task can be reduced to the diamagnetic Kepler problem. Finally in the system of atomic units the Hamiltonian of the considered problem takes the form:

\[
H = \frac{1}{2} p^2 - \frac{1}{r} + \frac{1}{8} \lambda (x^2 + y^2) = E, \tag{2.1}
\]

where \( \lambda = \frac{\hbar^3}{m_e^2 c^3} B \) is a constant describing the connection of the system with the external magnetic field. The form of the Hamiltonian (2.1) is similar to the one of (1.1). For \( \lambda = 0 \) the equations corresponding to (2.1) are integrable. For \( \lambda \neq 0 \) the system is nonintegrable. Finally with the increase of the amplitude of the magnetic field, starting with some definite value of \( \lambda c \), the dynamics appears to be chaotic. The use of the numerical methods for the Hamiltonian of the form (2.1) is connected with definite difficulties because of the appearance of singularity in the \( r = 0 \) point.

To get over this problem it is necessary to use semi-parabolic coordinates that are connected with the Cartesian ones via formulas:

\[
\begin{cases}
\mu = \sqrt{r + z} \\
\nu = \sqrt{r - z}
\end{cases}
\]

and make a transition to a non-homogeneous time via transformation \( dt = \left( \nu^2(\tau) + \mu^2(\tau) \right) d\tau \) [15]. Then taking into account that \( L_z = 0 \), the Hamiltonian (2.1) can be transformed to the following form [15]:

\[
\frac{1}{2} (p^2_\mu + p^2_\nu) - E(\mu^2 + \nu^2) + \frac{1}{8} \lambda \mu^2 \nu^2 (\mu^2 + \nu^2) = 2. \tag{2.2}
\]

I.e. the Hamiltonian is of form

\[
H(p_\mu, p_\nu, \mu, \nu, \lambda) = H_0(p_\mu, p_\nu, \mu, \nu) + \lambda V(\mu, \nu), \tag{2.2a}
\]

where \( H_0 = \frac{1}{2} (p^2_\mu + p^2_\nu) - E(\mu^2 + \nu^2) \) is the integrable part of the Hamiltonian; \( V = \frac{1}{8} \mu^2 \nu^2 (\mu^2 + \nu^2) \) is the nonintegrable part of the Hamiltonian.
Figure 1: Phase trajectory on the plane of variables \((\rho_\mu, \mu)\), obtained after the numerical integration of the Hamilton equations, corresponding to the Hamiltonian (2.2). The result (as all the other numerical calculations given in this work) is achieved by using the software MathWorks MatLab 6.0 for the values of parameters \(E = -0.125 \sim 10^{-19} J\), \(\lambda = 1.0\). As it is seen from the graph, the motion is of a chaotic type, and the destruction of the invariant tori points to this.

As one may see from (2.2a), the transformed Hamiltonian by its form coincides with the Hamiltonian of interacting oscillators, and in (2.2) the singularities which are typical for the Hamiltonian (2.1) are absent. Though one should take into account, that during the direct numerical calculations, right after the integration of the Hamilton equations corresponding to (2.2a), one has to perform a reverse transition to a real time.

Henceforth the transformed Hamiltonian will be the object of our investigations in case of classical consideration.

As it is clear from (2.2), the value of the magnetic field \(B\) is the parameter of nonlinearity. We shall study a case of a strong nonlinearity, i.e. the case when the methods of perturbation theory are inapplicable. In such case the chaos may appear in the system. We should expect to get a chaos in case of high magnetic fields \(B \geq B_c\).

When chaos appears, the mechanical concepts lose their meaning. For describing the processes taking place in the system, the statistical concepts: Kolmogorov entropy [7] and the fractal dimension of the phase space of the system [17–19] become significant. The study of the statistical features of the dynamical system can be performed only numerically.

The results of the numerical computations, gained by solving the Hamilton equations, corresponding to (2.2), are given in Fig.1 and Fig.2.

As seen from Fig.1 and Fig.2, the destruction of the invariant tori took place. The motion is of the chaotic type. For more convincing proof of the chaotic character of motion one has to perform Fourier analysis of the obtained
Figure 2: Phase trajectory on the plane of variables \((p_\nu, \nu)\) plotted under the conditions similar to the one in Fig. 1. The destructed invariant torus, according to KAM theorem [7], testifies to the existence of the classical chaos.

To define Kolmogorov entropy one has to perform a Fourier transformation of the correlation function

\[
G_\mu(\tau) = \langle \mu(t + \tau)\mu(t) \rangle, \\
G_\nu(\tau) = \langle \nu(t + \tau)\nu(t) \rangle, \\
G(\omega) = \int G(\tau)e^{i\omega \tau}d\tau = \frac{\tau_c}{1 + \omega^2 \tau_c^2},
\]

(2.3)

where

\[
\langle (\cdots) \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T (\cdots)dt,
\]

means averaging over the time, \(\tau_c\) is the correlation time, connected with the Kolmogorov entropy by the ratio \(h_0 \sim \frac{1}{\tau_c}\). In practical calculations of (2.3) it is more convenient to use a realization of a Fast Fourier Transform algorithm [20, 21]. As the numerical calculations show, the value of the correlation time is \(\tau_c \sim 10^{-15}s\). The results of numerical calculations are presented in Fig. 3.

There is one more interesting property of dynamical systems connected with the Kolmogorov entropy that describes chaotic motion and is called Poincaré recurrence. The main point of the Poincaré recurrence is that any system with a finite phase space after some definite time returns to its initial state [22]. The study of the time of Poincaré recurrence is one of the most powerful methods of the analysis of the nonlinear systems.

It turned out to be that in conditions of strong chaos (i.e. when the phase plane doesn’t contain the stability islands) the distribution of the times of
The dependence of the Fourier image of the correlation function \( G_\mu(\omega) \) on the frequency \( \omega \) (10\(^{15}\) Hz), plotted using Eq. (2.3) and FFT method. The presence of the finite width of the correlation function \( G_\mu(\omega) \) is the evidence of the appearance of chaos. In other words, one may say, that oscillatory process is not characterized by a definite frequency (period). All the frequencies (periods) in a finite frequency interval \( \delta \omega \sim 1/\tau_c = 200THz \) are involved into oscillatory process.

Poincaré recurrences has a Lorenz structure [22]:

\[
P(\tau) = \frac{1}{\tau_{rec}} \exp(-\tau/\tau_{rec}),
\]  

(2.4)

where \( \tau_{rec} = \int_0^\infty \tau P(\tau)d\tau \) is the average recurrence time connected with Kolmogorov entropy as \( \tau_{rec} = \frac{1}{\delta_\theta} \). Thus, calculating the value of the Kolmogorov entropy one can define the distribution of the recurrence times.

We in details touched upon the question about classical Poincaré recurrences, because henceforth we will be interested in quantum Poincaré recurrences. The idea of quantum Poincaré recurrence was introduced in the recently published work by G. M. Zaslavsky and A. Iomin [22]. We shall return to the description of this phenomenon during a quantum consideration.

One of the signs of the appearance of chaos is a discrete (fractal) dimension of the phase space of the system.

For estimation of the fractal dimension we shall use the Grassberger-Procaccia algorithm [17–19]. The main point of this algorithm consists into following:

Assume we have obtained from a numerical solution of the equations of motion a set of state vectors \( \{ x_i, i = 1, 2, \cdots, N \} \) that correspond to the sequential steps of integration. In our case \( x_i \) denote a complete set of variables, characterizing the phase space of the system: \( P_\mu(t_i), P_\nu(t_i), \mu(t_i), \nu(t_i), t_1 = 0, t_N = T \), where \( t_i \in [0,T] \) is the time interval for the numerical integration. Defining...
some (small) $\epsilon$, we can use our set for estimation of the following sum:

$$C(\epsilon) = \lim_{N \to \infty} \frac{1}{N(N-1)} \sum_{i,j=1}^{N} \theta(\epsilon - |x_i - x_j|),$$

where $\theta$ is the Heaviside step function

$$\theta(x) = \begin{cases} 
0, & x < 0, \\
1, & x \geq 0.
\end{cases}$$

According to Grassberger-Procaccia algorithm, if one knows $C(\epsilon)$, the fractal dimension of the strange attractor may be defined

$$D = \lim_{\epsilon \to 0} \frac{C(\epsilon)}{\log(\epsilon)}.$$ 

One should calculate $C(\epsilon)$ for different values of $\epsilon$ and represent the results in coordinates $\log(\epsilon)$ and $\log(C(\epsilon))$.

The expected dependence of $C(\epsilon)$ has a form of $\epsilon^D$, so that the obtained graph must have a straight-line form with $D$ angular coefficient. Results of the numerical calculations are presented in Fig.4 and Fig.5.

3 Quantum Consideration

As it has been already mentioned, usually the quantum chaos is considered as a set of phenomena that appear in quantum systems, the classical analogues of
Figure 5: Graph of the dependence of $C(\epsilon)$ on $\epsilon$, plotted in a logarithmic scale using the Grassberger-Proccacia algorithm [17–19]. The graph is plotted via the integration of classical Hamilton equations corresponding to the Hamiltonian (2.2) for the values of parameters $E = -0.125 \sim 10^{-19} J$, $\lambda = 1.0$. The curve line corresponds to the results of the numeric data. The straight-line is plotted via the processing of the numerical data with least squares algorithm. From this graph one can estimate the fractal dimension of the attractor using the formula $D = \frac{\log(C(\epsilon_2)) - \log(C(\epsilon_1))}{\log(\epsilon_2) - \log(\epsilon_1)} \approx 2.857$.

which display chaos. The difficulty in definition of quantum chaos is connected with a fact, that the concepts characterizing classical chaos (local instability of phase trajectories) lose their sense in quantum consideration. Therefore, for describing quantum chaos one has to use methods and concepts which are typical for quantum mechanics.

Our goal in case of quantum consideration, is the demonstration of the fact that one of the signs of the quantum chaos is a formation of the mixed state. For endorsement of this assumption we shall use methods of random matrix theory [1, 28, 29]. Due to this fact, we have to use basis of eigenfunctions of the integrable part of the Hamiltonian (2.1) and we cannot expend the wave function in Landau states, as was done in [15]. This makes situation more complicated but as we are interested in the state $l = 0, m = 0$, some analytical results still can be obtained.

Let us write down the Schrödinger equation for the Hamiltonian (2.1)

$$\hat{H}(\vec{p}, \vec{r}, \lambda)|\psi(\vec{r}, \lambda)\rangle = E(\lambda)|\psi(\vec{r}, \lambda)\rangle. \tag{3.1}$$

It is easily seen from (3.1), that the Schrödinger equation in contrast to the classical equations of Hamilton is linear. Like in the case of classical systems, this conclusion means that Eq.(3.1) is completely deterministic and does not contain the properties of chaos, the main sign of which is fortuity and abruptness of the behavior of system. Because of this the question appears: Then how can one observe nonregular behavior and quantum chaos in the quantum
systems? To answer this question we shall use some well-known facts from quantum mechanics [23,24,25].

Let us define via $|\psi_n(\vec{r},\lambda)\rangle$ the required eigenfunction of the Eq. (3.1) and expand it in eigenfunctions of the Hamiltonian $\hat{H}(\vec{p}, \vec{r}, 0) = \hat{H}_0(\vec{p}, \vec{r})$

$$|\psi_n(\vec{r},\lambda)\rangle = \sum_m C_{nm}(\lambda)|\Phi_m(\vec{r})\rangle.$$  

(3.2)

Here $|\Phi_m(\vec{r})\rangle$ is the eigenfunction of the Hamiltonian $\hat{H}_0(\vec{p}, \vec{r})$.

According to the universally recognized rules of quantum mechanics, the coefficients of the expansion $C_{nm}(\lambda)$ taken squared by module, define the probability to find the considered system in state described by wave-function $|\Phi_m(\vec{r})\rangle$, and that is why they satisfy the conditions of normalization:

$$\sum_m |C_{nm}(\lambda)|^2 = 1.$$  

(3.3)

Substituting the expansion (3.2) into Schrödinger equation (3.1), one can obtain a matrix equation for $C_{mn}$

$$\sum_p H_{kp}C_{pn} = E_nC_{kn}(\lambda),$$  

(3.4)

where the elements of matrix $H_{kp}$ are defined by the integrals of the type:

$$H_{kp} = \langle \Phi_k(\vec{r})|\hat{H}(\vec{p}, \vec{r}, \lambda)|\Phi_p(\vec{r})\rangle.$$  

(3.5)

It is shown in quantum mechanics [23-25] that the series (3.2) exactly converges to the function $|\psi_n(\vec{r},\lambda)\rangle$, if when taking sum by $m$ a totality (infinite number) of functions $|\Phi_m(\vec{r})\rangle$ is considered. However the wave function $|\psi_n(\vec{r},\lambda)\rangle$ from a qualitative point of view may be with a high degree of accuracy described by the expansion like (3.2) using a finite number $N$, ($N >> 1$) of states $|\Phi_m(\vec{r})\rangle$. The further increase of the number of states $N$ is similar to the tendency of the Planck constant to zero $\hbar \rightarrow 0$ and leads to the improvement of quantitative fit between classical and quantum chaos [4, 5].

According to the premises one may say, that the problem of finding eigenfunctions and eigenvalues of Hamiltonian $\hat{H}(\vec{p}, \vec{r}, \lambda)$ may be solved by a numeric diagonalization of the matrix equation (3.4).

But here a question is born. If the state of the system is described by a finite superposition of regular states $|\Phi_m(\vec{r})\rangle$, then the state $|\psi_n(\vec{r},\lambda)\rangle$ is regular too, so where should one look for a nonregular behavior of the system?

By the assumption taken for today [1,28,29] the properties of chaos in quantum system are revealed in that sense that matrix (3.5) is a random matrix, all the elements of which are random values. Based on this, there must exist some correspondence between matrix (3.5) and the quantities describing classical chaos. Using our problem as a pattern we shall start to examine this question.
Let us start with quantum mechanical investigation of the Hamiltonian (2.2). As it has been already mentioned, when the external magnetic field is absent $\lambda = 0$ the Hamiltonian $\hat{H}(\vec{p}, \vec{r}, 0)$ is exactly integrable. When the external magnetic field is turned on $\lambda > 1$ the Hamiltonian becomes nonintegrable, and for some definite value $\lambda = \lambda_0$ the solutions of the classical equations corresponding to the Hamiltonian $\hat{H}(\vec{p}, \vec{r}, \lambda_0)$ display chaos. By analogy with classical chaos, when a set of phase trajectories with a small dispersion of initial conditions is investigated, we shall consider a small increment of the parameter $\delta \lambda = \lambda - \lambda_0$. Using the basis of functions in which Hamiltonian $\hat{H}(\vec{p}, \vec{r}, \lambda_0)$ is diagonal, for small values of $\delta \lambda$ the Hamiltonian $\hat{H}(\vec{p}, \vec{r}, \lambda)$ may be represented as a sum of two matrices:

$$\hat{H} = E_0 + \delta \lambda B,$$

where $E_0$ is a diagonal matrix, $B$ is a banded matrix, the elements of which are random numbers. By a numerical diagonalization, one can define the eigenfunctions $|\psi_n(\vec{r}, \lambda + \lambda_0)|$, $|\psi_n(\vec{r}, \lambda)|$, and eigenvalues $E_n(\lambda_0 + \delta \lambda_0)$, $E_n(\lambda_0)$ corresponding to the $\hat{H}(\vec{p}, \vec{r}, \lambda)$ and $\hat{H}(\vec{p}, \vec{r}, \lambda_0)$ respectively. We are interested in the interval of energy $\delta E = E(\lambda_0 + \delta \lambda_0) - E(\lambda_0)$ which is small from a classical point of view, and large from a quantum mechanical one (with relation to the large number of quantum levels contained in this interval).

Let us begin to the quantum mechanical analysis of the Hamiltonian (2.1). The eigenvectors of the basis, in which Hamiltonian is diagonal, can be found easily and are of the form [23]

$$|\Phi_{n,l,m}(r, \theta, \varphi)\rangle = |R_{nl}Y_{lm}(\theta, \varphi)\rangle, \quad (3.7)$$

where $R_{nl} = \frac{2}{n^{l+2}}(2l+1)\sqrt{\frac{(n+l)!}{(n-l-1)!}}(2n)^{l/2}e^{-r^2/4}F(-n + l + 1, 2l + 2, \frac{2r}{n})$ is the normalized radial part of the wave function and $Y_{lm}(\theta, \varphi)$, $F(-n + l + 1, 2l + 2, \frac{2r}{n})$ are the spherical and hyper-geometrical functions respectively [27]; $r$, $\theta$ and $\varphi$ denotes the spherical coordinates.

As was mentioned above, using of the symmetric Kepler problem’s eigenfunctions is connected to the requirements of the random matrix theory. Calculation of non-diagonal matrix elements in this basis is more complicated than in Landau basis [15,23]. But the fact that we are interested in the state $l = 0$, $m = 0$ makes life and it’s still possible to obtain some analytical results. Actually the problem is reduced to the calculation of the following matrix elements:

$$\langle \Phi_{n,0,0}(r, \theta, \varphi)|x^2 + y^2|\Phi_{m,0,0}\rangle = \langle \Phi_{n,0,0}(r, \theta, \varphi)|r^2\sin^2\theta|\Phi_{m,0,0}(r, \theta, \varphi)\rangle. \quad (3.8)$$

These matrix elements can be calculated analytically. As a result for diagonal matrix elements we get [25]:

$$\langle \Phi_{n,0,0}(r, \theta, \varphi)|r^2\sin^2\theta|\Phi_{n,0,0}\rangle = \frac{n^2}{2}(5n^2 + 1) \quad (3.9)$$

and non-diagonal matrix elements can be reduced to the calculation of the following integral:

$$\langle \Phi_{n,0,0}(r, \theta, \varphi)|r^2\sin^2\theta|\Phi_{m,0,0}(r, \theta, \varphi)\rangle = \frac{1}{3n^{3/2}m^{3/2}}J^{S,0}_{\gamma}(\alpha, \alpha'), \quad (3.10)$$
\[ J^{S,0}_\gamma (\alpha, \alpha') = \int_0^\infty e^{-\frac{k + k'}{2}} F(\alpha, \gamma, kr) F(\alpha', \gamma, k'r) dr, \]

where
\[ k = \frac{2}{n}; k' = \frac{2}{m}; \alpha = -n + 1; \alpha' = -m + 1; \gamma = 2; S = 3. \]

Direct calculation of the integral \( J^{S,0}_\gamma (\alpha, \alpha') \) is not possible. But we can use recurrence formula, which connects integral \( J^{S,0}_\gamma (\alpha, \alpha') \) and integrals with the lower values of superscript \( J^{S-1,0}_\gamma (\alpha, \alpha') \); \( J^{S-2,0}_\gamma (\alpha, \alpha') \). After straightforward but laborious calculations one can obtain \( J^{S,0}_\gamma (\alpha, \alpha') \):
\[
J^{S,0}_\gamma = \frac{4}{k'^2 - k^2} \left[ \left( \frac{\gamma}{2} (k - k') - k\alpha + k'\alpha' - k'(S - 1) \right) J^{S-1,0}_\gamma (\alpha, \alpha') + 
+ (S - 1) (\gamma - 1 + S - 1 - 2\alpha') J^{S-2,0}_\gamma (\alpha, \alpha') + 2\alpha' (S - 1) J^{S-2,0}_\gamma (\alpha, \alpha' + 1) \right]
\]
where
\[
J^{0,0}_\gamma (\alpha, \alpha') = 2^\gamma \Gamma(\gamma)(k + k')^{\alpha + \alpha'} - \gamma(k' - k)^{-\alpha}(k - k')^{-\alpha'} F(\alpha, \alpha', \gamma, -\frac{4kk'}{(k - k')^2})
\]
and \( \Gamma(\gamma) \) is the Euler gamma function \([27]\).

4 \textbf{Irreversible evolution of the quantum chaos.}

\textbf{Formation of the mixed state.}

At the discussion of the nonreversible evolution of the quantum -mechanical system, naturally the question emerges. How in a quantum system originates non-reversibility? If the quantum system evolves according to the Schrödinger equation, how can a pure quantum -mechanical state become a mixed one? The question is that, in contrast to the classical chaos, quantum mechanically irregular motion cannot be characterized by extreme sensitivity to tiny changes of the initial data. Due to the unitarity of the quantum dynamics, the overlap of two wave functions remains time-independent \(|\langle \vartheta(t) | \zeta(t) \rangle|^2 = |\langle \vartheta(0) | \zeta(0) \rangle|^2\), provided time-dependence of \( \vartheta(t) \) and \( \zeta(t) \) is generated by the same Hamiltonian. However, an alternative characterization of classical chaos, extreme sensitivity to slight changes of the dynamics does carry over into quantum mechanics.

Let us assume, that the amplitude of the external magnetic field is modulated by varying field
\[ B = B_0 + \Delta B_0 \cos \Omega t. \]

Taking into account (4.1) the Schrödinger equation for the wave function of diamagnetic hydrogen atom takes the form
\[
\frac{i\hbar}{\partial t} |\psi(r, \lambda(t))\rangle = \hat{H}(t) |\psi(r, \lambda(t))\rangle,
\]
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where
\[ \hat{H}(t) = \hat{H}_0(\vec{p}, \vec{r}, \lambda_0) + \Delta \lambda(t) V(r, \theta), \]
\[ \Delta \lambda(t) = \Delta \lambda \cos \Omega t. \]

The solution of the time-dependent Schrödinger equation formally can be written with the help of a time-ordered exponential
\[ U(t) = \{ \exp[-\frac{i}{\hbar} \int_0^t dt' \hat{H}(t')] \}_+, \]
where the positive time ordering requires
\[ [A(t)B(t')]_+ = \begin{cases} A(t)B(t') & \text{if } t > t' \\ B(t')A(t) & \text{if } t < t' \end{cases}. \]

In our case \( H(t + \frac{2\pi k}{\Omega}) = H(t), \) the evolution operator referring to one period \( T_0 = \frac{2\pi}{\Omega}, \) the so-called Floquet operator \( U(T_0) \equiv \hat{F} \) [1], is worthy of consideration since it yields a stroboscopic view of the dynamics
\[ \psi(kT_0) = (\hat{F})^n \psi(0). \quad (4.3) \]

The Floquet operator, being unitary, has unimodular eigenvalues. Suppose we can find eigenvectors \( |\varphi_\chi\rangle \) of the Floquet operator
\[ \hat{F}|\varphi_\chi\rangle = e^{-i\varphi_\chi}|\varphi_\chi\rangle, \quad (4.4) \]
\[ \langle \varphi_\chi | \varphi_\theta \rangle = \delta_{\chi \theta}. \]

Then, with the eigenvalue problem solved, the stroboscopic dynamics can be written out explicitly [1]
\[ \psi(kT_0) = \sum_\chi e^{-ik\varphi_\chi} \langle \varphi_\chi | \psi(0) \rangle |\varphi_\chi\rangle. \quad (4.5) \]

As it was mentioned above, our aim is to proof that one of the signs of the emergence of quantum chaos is a formation of the mixed state. Being initially in a pure quantum mechanical state, described by the wave function \( \psi_n, \) the system during the evolution makes an irreversible transition to the mixed state.

After the formation of a mixed state the quantum-mechanical description loses its sense and we have to use a quantum-statistical interpretation. To prove the formation of the mixed state, one has to show the zeroing of non-diagonal elements of density matrix, the equality of which to zero is a sign of a mixed state [30, 31].

Taking (4.5) into account, we obtain for non diagonal matrix elements of the density matrix:
\[ \rho_{nm} = C_n^* C_m, \quad (4.6) \]
where \( C_n = e^{-ik\varphi_n} \langle \phi_n | \psi(0) \rangle, \) \( \langle ... \rangle \) means averaging over time.
For averaging let us recollect that value $\phi_n$ is the eigenvalue of the Floquet operator. Owing to the non-integrability of the system, eigenvalues can be obtained only by way of numerical diagonalization of the Hamiltonian $\hat{H}$ (4.2). According to the main hypothesis of the random matrix theory [1,11], elements of this matrix in the chaotic domain are random values. So, their eigenvalues also can be considered as random values. This statement is valid only in the chaotic domain [32]. According to this, the phase

$$f(n,m) = \phi_m - \phi_n,$$  

(4.7)

also may be considered as random. Therefore when $T = kT_0$, $k \gg 1$, we get

$$\rho_{nm} = \frac{T_0}{T} \sum_{k=1}^{T/T_0} (e^{-ikf(n,m)}) \langle \phi_m | \psi(0) \rangle \langle \psi(0) | \phi_n \rangle = 0,$$  

(4.8)

where $\langle ... \rangle$ denotes ensemble average of random matrices, that corresponds to a small dispersion of the value of magnetic field parameter $\delta \lambda_0$.

Expression (4.8) may be found by more vigorous mathematical substantiation. For this let us recall some details from the probability theory [33].

a) In general case, under the characteristic function of the random value $X$, mathematical expectation of the following exponent is meant

$$F(t) = M(\exp(itX)),$$  

(4.9)

where $t$ is a real parameter.

b) Mathematical expectation itself is defined as a first moment $\mu_1$ of the random variable $X$

$$M(X) = \langle X \rangle = \mu_1 = \sum_k x_k P_k,$$  

(4.10)

where $X$ is the discrete random variable which takes possible values $x_1, x_2, ...$ with appropriate probabilities $P_k = P(X = x_k)$, $\langle ... \rangle$ means average.

Taking (4.9), (4.10) into account and considering $f(n,m)$ as a random value, we get:

$$\rho_{nm} = \frac{T_0}{T} \sum_{k=1}^{T/T_0} F(k),$$  

(4.11)

where

$$F(k) = M(e^{ikf(n,m)}),$$  

(4.12)

is the mathematical expectation of the characteristic function of the random phase $f(n,m)$, and

$$A = \langle \phi_m | \psi(0) \rangle \langle \psi(0) | \phi_n \rangle.$$

Let us assume that random phase $f(n,m)$ has a normal dispersion [33]. Then from (4.12) one can obtain

$$F(k) = e^{iak} e^{-\frac{k^2 \sigma^2}{2}},$$  

(4.13)
where
\[ a = M(f(n,m)), \quad (4.14) \]
is the mathematical expectation of the random phase,
\[ \sigma^2 = M(f^2(n,m)) - (M(f(n,m)))^2, \quad (4.15) \]
is the mean square deviation.

Substituting (4.13) in (4.11) and making transition from summation to the integration \( \sum_k \to \int dk \) finally we get
\[ \rho_{nm}(T) = \frac{C_0}{T} \left( \text{Erfi} \left[ \frac{a}{\sqrt{2}\sigma} \right] + \text{Erfi} \left[ \frac{a + i(T/T_0)\sigma^2}{\sigma} \right] \right), \quad (4.16) \]
where \( C_0 = iAe^{\frac{-a^2}{2\sigma^2}} \) and \( \text{Erfi}(... \right) \) is the error function, connected to the ordinary error function [33] by the relation
\[ \text{Erfi}(x) = -i\frac{\sqrt{\pi}}{2} \text{Erfi}(ix). \quad (4.17) \]

Taking into consideration asymptotical form of the function \( \text{Re}(\text{Erfi}(x)) \to 0, \quad x \to \infty \) and \( \text{Im}(\text{Erfi}(x)) \to 1, \quad x \to \infty \), in case when distribution of the eigenvalues of the quantum-mechanical chaotic system obeys the normal distribution, we have
\[ |\rho_{nm}(T)| \sim \frac{1}{T} \sim 0, \quad T \gg T_0. \quad (4.18) \]

Zeroing of the non-diagonal elements of density matrix is the sign of quantum chaos beginnings and formation of mixed state. From that moment the quantum dynamics is non-reversible since the information about the wave functions phase is lost. Given above reasoning can be checked by numerical experiment, which consists in: the direct solving of non-stationary Schrödinger equation (4.2), defining eigenvalues \( \varphi_\lambda \) and in estimation of the averaged non-diagonal elements of the density matrix according to (4.8).

The result of numerical calculations is represented on Fig.6.

5 Quantum Poincaré Recurrences

According to the results of the previous section (see Fig.6), for times \( t > \tau_c \) formation of a mixed state happens due to time evolution of quantum-mechanical system. Consequently the concept of a wave function loses its meaning and the Poincaré recurrences are out of the question. But what happens when \( t < \tau_c \)?

We shall clear up this question in the given section.

As it was mentioned above, in work [22] the concept of quantum Poincaré recurrence was introduced. In particular, the authors have studied the quantum dynamics of one-dimensional rotator under the influence of delta-like perturbation. The definition of the "distance" between the wave-functions was
Figure 6: The graph of the dependence of the second term $\rho_{mn}$ of non-diagonal matrix element (4.6) on time $t = kT_0$. The graph is obtained using (4.8) and by way of numerical diagonalization of the Hamiltonian (4.2) for different values $H(t_i) = H(\lambda(t_i))$, $t_i \in [0, T]$. The graph is plotted after taking an ensemble average of Hamiltonians $H(\lambda_0)$, corresponding to the dispersion $\delta \lambda_0 = 0.1$ of the value of magnetic field $\lambda_0$. As it is easily seen from the graph that when $t = kT_0 > \tau_c$, $T_0 = \frac{\pi}{\Omega} = 0.1\tau_c$, zeroing of $\rho_{nm}$ happens. In the numeric calculations we have used definite initial conditions $\psi_n(0), \psi_m(0)$, obtained via numerical diagonalization of the Hamiltonian (2.1) for $\lambda_0 = 1$. The dimension of the diagonalized matrix was $500 \times 500$, $\chi, \zeta = 1, 500$.

introduced

$$d^2(t) = \langle \Psi(\vec{r}, t) - \Psi(\vec{r}, 0) | \Psi(\vec{r}, t) - \Psi(\vec{r}, 0) \rangle,$$

where $|\Psi(\vec{r}, t)\rangle$ is the solution of nonstationary Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}(t)\Psi.$$  

(5.2)

The authors of the work, cited above, look for the solution of the equation (5.2) in the form of expansion of the function $|\Psi(\vec{r}, t)\rangle$ in an arbitrary orthogonal basis $|\Phi_m\rangle$

$$|\Psi(\vec{r}, t)\rangle_n = \sum_m C_{nm}(t) |\Phi_m(\vec{r})\rangle,$$

(5.3)

where $C_{nm}(t)$ are the expansion coefficients, which determine the time dependence of the function $|\Psi(\vec{r}, t)\rangle_n$. It is obvious, that during the evolution in time of the wave-function $|\Psi(\vec{r}, t)\rangle$, the quantity $d(t)$ will change in time. The authors offer to consider the quantum Poincaré recurrences as such values of time $t$, that satisfy the condition $|d(t)| < \epsilon$, where $\epsilon$ is a small constant value ($\epsilon < 1$).

Our purpose is the use of this method for the study of quantum Poincaré recurrences in the system of diamagnetic hydrogen atom. For that, like in the previous section, we shall assume, that the amplitude of the external magnetic
Figure 7: The histogram of distributions of the times of quantum Poincaré recurrences, plotted in compliance with the definition (5.1). The quantity $N(\tau)$ determines the dependence of the number of quantum Poincaré recurrences on the distribution of the periods of recurrences. $\lambda_0 = 1$, $\Delta \lambda = 0.1$, $\Omega = \frac{2\pi}{T_0}$, $T_0 \sim 0.1 \tau_c \approx 0.5 \cdot 10^{-15} \text{s}$.

Field is modulated by a varying field. But in contrast to the previous section, we shall examine the solution of the equation in interval $t < \tau_c$, when the system is still in a pure quantum-mechanical state and chaotization of phase and formation of a mixed state can be neglected.

Before starting the analysis of the equation (4.2), let us note some typical differences of our problem from the problem studied in [22]. In problem studied in [22], the dimension of the Hilbert space is finite. That is why the wavefunction $|\Psi(\vec{r},t)\rangle_n$, according to (5.3), is exactly defined by the finite set of the orthogonal functions $|\Phi_m(\vec{r})\rangle$. The authors make an assumption, that the expansion coefficients $C_{nm}(t)$ are the random quantities and satisfy the Gaussian distribution.

In our case the dimension of the Hilbert space is infinite and the approximation of $|\Psi(\vec{r},t)\rangle_n$ by the finite set of functions of the orthogonal basis $|\Phi_m(\vec{r})\rangle$ is rough. Our purpose is a proof that in spite of it the quantum Poincaré recurrences may happen in the system.

For the solution of the nonstationary Schrödinger equation (4.2) we shall consider $t$ as a discrete quantity (consequently the values of the parameter $\delta\lambda(t)$ become discrete too). We shall not assume the coefficients $C_{nm}(\lambda,t)$ to be \emph{a priori} random, but we shall determine their values by solving the matrix equation (3.5) and taking into account the dispersion of the parameter $\delta\lambda_0$. Thus, using the formulas (3.2), (3.5) and (5.1) one can define the distribution of the times of Poincaré recurrences. The results of numeric calculations are shown in Fig.7 and Fig.8.

According to Fig.8, the distribution of the times of Poincaré recurrences is of the Lorenz form. This fact can be easily explained, taking into account the
Figure 8: Exponential approximation of the numeric data represented in Fig.7, made in compliance with the formula (2.4). The graph is plotted in a logarithmic scale. Therefore a straight line on the given graph corresponds to the exponential Lorentz form. The result allows to determine numerically the mean time of quantum Poincaré recurrences $\tau_{\text{rec}}^Q$ and to compare it with the mean time of classical Poincaré recurrences $\tau_{\text{rec}} \sim \tau \sim 1/\hbar_0$ (see formula (2.4)). As it comes from the graph, $\tau_{\text{rec}}^Q \sim \frac{1}{|b|} \approx 0.5 \cdot 10^{-14}$s, where $b$ is the angular coefficient of the approximating straight-line. The achieved estimate for the mean time of quantum recurrences is in a good agreement with the mean value of the classical Poincaré recurrences $\tau_{\text{rec}} \sim \tau_C \sim \frac{1}{2\pi} = 0.5 \cdot 10^{-14}$s (see Fig.3).

existence of a strong classical chaos (i.e. the absence of the stability islands in the phase space).

The Lorentz form testifies that if $t > \tau_{\text{rec}}^Q = \tau_C$, quantum Poincaré recurrences are improbable. This coincides with the results of the previous section, according to which the system is found in a mixed state in this time interval.

Based on the results obtained above, one may assert that quantum Poincaré recurrences also take place in quantum systems with infinite ”phase space” (i.e. with infinite-dimensional Hilbert space).

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