# Bohr billiard: Decay in the chaotic Hamiltonian system with two integrals of motion

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The two-dimensional system of two identical hard disks moving freely within the circular potential well (billiard) of finite depth is studied as an example of the Hamiltonian chaotic system with two integrals of motion—the total energy and the total angular momentum. The kinetics of decay in the ensemble of such systems with fixed values of integrals of motion can be described by the exponential law, if the energy is lower than the threshold of two-particle decay. For this range the rate of the decay is calculated analytically as a function of energy, angular momentum, and the ratio of disk and billiard radii. The numerical calculations confirm the theoretical estimate of the decay rate in the wide range of its values. [S1063-651X(97)12810-0]

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## I. INTRODUCTION

In this paper we investigate the Hamiltonian chaotic system of two particles in an external potential, which can be treated as a round billiard with two hard disks moving freely within it.

Similar models were introduced repeatedly but they never have been thoroughly investigated. To explain the fast neutron capture by some nuclei, Bohr in 1936 introduced the model of hard spheres moving in a two-dimensional potential well [1,2]; see Fig. 1. Bohr has qualitatively analyzed the dynamics of the system in the case when one fast sphere enters into the well that confines some large number of spheres. The energy redistribution between the spheres makes the time of decay of the system much larger than the time of free passage of the incoming sphere through the well. The model served to illustrate the process under consideration. Since quantum effects are crucial for a realistic description of nuclei, the quantitative analysis of the classical model, which we shall call *the Bohr billiard*, has not been attempted.

The second avatar of the model was related to the ergodic theory. In this context Sinai has investigated some models similar to the Bohr billiard. In 1963 he proved the ergodicity of motion for the Sinai billiard [3,4], consisting of a particle moving freely in a plane within the domain of a certain form, shown in Fig. 2, bordered by rigid walls. This discovery has been developed into the theory of one-particle chaotic billiards, which now plays an important role in chaotic dynamics [5–9]. Some attempts to extend the main results for more complicated system have been carried out [10], but in general many-particle models have received no attention again.

Our model of the Bohr billiard can serve different purposes. First, it has four degrees of freedom with unambiguously and exactly defined energies. The process of accumulation of energy in one degree of freedom, which turns eventually into the channel of decay, is important in the theory of unimolecular reactions [11]. The Bohr billiard accounts for strong repulsion of particles at small distances. This type of interaction is inherent, for example, to models of rare-gas clusters with Lenard-Jones potential of pairwise interaction. Usually the process of decay of clusters is described by Rice-Ramsperger-Kassel (RRK) theory [12]. The complementary approach can be provided by the Bohr billiard model and its generalization to three dimensions and a larger number of particles.

Secondly, the model has two integrals of motion—the total energy and the component of the total angular momentum orthogonal to the billiard plane (in what follows for brevity it will be called the angular momentum). Hence, the motion is not ergodic on the energy surface, and the question of structure of invariant manifolds of the system's phase space arises.

Thirdly, high energy states of the Bohr billiard can be studied in the paradigm of the theory of irregular scattering [13-17]. The model allows one to study the problems of irregular scattering of particles on targets with internal degrees of freedom. These problems, which form the next level in comparison with the problems of potential irregular scattering, are of great interest for the theory of chemical reactions and have been approached recently [16,17].

In this paper special attention is given to Bohr's original problem of the kinetics of the decay of a system in high energy states, for which the escape of particles to infinity is possible. The stationary distributions of values of some dynamical variables are found for the bound states. They are used as tools for studying the problem of decay. The characteristics of chaotic motion in the bound states were studied only to the extent that gave sufficient support to main approximations used in the theory of decay.

The remainder of the paper is organized as follows. The model and its characteristic parameters are described in Sec.







FIG. 2. The Sinai billiard is a part of plane limited by sides of the square (with length *a*) and a concentric circle (with radius *R*). The particle moves freely within the billiard and reflects elastically from its wall: the dashed line shows a part of a trajectory. For any finite value of R/a the motion of the particle is ergodic.

II. The properties of the bound states of the system—the distributions of dynamical variables and their correlation functions—are studied in Sec. III. In Sec. IV we derive the theoretical estimate of the dependence of the decay rate of highly excited states of the Bohr billiard on the energy and the angular momentum of the system and its geometry. The numerical studies of the decay are described in Sec. V. Section VI presents the comparison of the theoretical and numerical results and the general discussion.

### **II. THE MODEL**

The Bohr billiard can be defined as a two-particle system in the external field with the Hamiltonian function

$$H = \sum_{i=1}^{2} \left[ \frac{p_i^2}{2m} + U(\mathbf{r}_i) \right] + V(r_{12}).$$
(1)

Here  $\mathbf{r}_i$  and  $\mathbf{p}_i$  are two-dimensional vectors of position and momentum of the *i*th particle, *m* is the particle mass,  $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ . The particle interaction is described by the hard disk repulsion potential

$$V(r_{12}) = \infty$$
  $(r_{12} < 2a), V(r_{12}) = 0$   $(r_{12} > 2a),$  (2)

where *a* is the disk radius (see Fig. 3). The external field potential  $U(\mathbf{r}_i)$  is given by the circular potential well of finite depth,

$$U(\mathbf{r}_{i}) = 0$$
  $(r_{i} < A - a), \quad U(\mathbf{r}_{i}) = U_{0} \quad (r_{i} > A - a),$ 
(3)

where A is the billiard radius. The circle  $r_i = A - a$  will be called the billiard wall. The geometry of the system can be characterized by the dimensionless parameter  $\alpha = a/(A - a)$ , which has values in the range  $0 < \alpha < 1$ .

The total energy E and the total angular momentum

$$\Lambda = \left| \sum_{i=1}^{2} \left[ \mathbf{r}_{i} \times \mathbf{p}_{i} \right] \right| \tag{4}$$

are the integrals of motion of the system. For a given value of E values of  $\Lambda$  cannot exceed the limit

$$\Lambda_{+} = 2(A-a)\sqrt{mE}.$$
(5)



FIG. 3. The Bohr billiard. The disks move freely within the circular potential well of the finite depth, colliding elastically with the wall and with each other. The total energy and the total angular momentum of the system are conserved quantities.

The mechanical state of the system can be characterized by two dimensionless parameters:

$$u = \frac{U_0}{E}, \quad L = \frac{\Lambda}{\Lambda_+}.$$
 (6)

The system is in a bound states if u > 1 or if u < 1 and  $L > \sqrt{1-u}$ ; then the particles are located within the billiard for all moments of time. If u < 1 and  $L < \sqrt{1-u}$ , the system is in a decay state: one or two particles can leave the billiard and escape to infinity. The value  $L_b = 1/\sqrt{2} = 0.707$  is an important threshold: for  $L > L_b$  both particles have angular momenta of the same sign.

In what follows values m, A-a, and 2E will be used as units of mass, length, and energy, respectively. The mechanical states of the system will be described by the following eight dynamical variables: the absolute value of momentum of the *i*th particle  $p_i$ , its angular momentum  $l_i$ , polar angle of its position  $\varphi_i$ , and the angle between the polar radius and the momentum direction  $\theta_i$  (everywhere i=1,2). It should be noted that the polar radii of particles are not included in this set.

The energy and angular momentum conservation laws now can be expressed in the form

$$p_1^2 + p_2^2 = 1 - Nu, \quad l_1 + l_2 = L,$$
 (7)

where N is the number of particles outside the billiard. Equation (7) defines the six-dimensional surface S in the eight-dimensional phase space of the Bohr billiard.

If we use  $p_1, l_1, \varphi_{1,2}, \theta_{1,2}$  as independent coordinates on the surface S, then  $p_2$  and  $l_2$  are determined by the Eq. (7) with N=0. The measure dM of the elementary part of the surface S is written as

$$dM = \frac{J}{\sqrt{1 - \Phi^2}} dp_1 dl_1 d\theta_1 d\theta_2 d\varphi_1 d\varphi_2, \qquad (8)$$

where J is Jacobi determinant

$$J = \frac{D(x_i, y_i, p_{xi}, p_{yi}; i=1,2)}{D(p_i, l_i, \theta_i; \varphi_i; i=1,2)} = \frac{2l_1l_2}{p_1p_2 \sin^2\theta_1 \sin^2\theta_2} \quad (9)$$

and the geometric factor  $(1-\Phi^2)^{-1/2}$  accounts for the relative directions of the normal to the surface *S* and the gradient of independent coordinates:

$$\Phi^2 = \sum_{j=1}^{6} (\mathbf{n} \cdot \mathbf{e}_j)^2, \qquad (10)$$

where **n** is the six-dimensional unit vector of the external normal to *S*, and  $\mathbf{e}_j$  is the unit vector in the direction of the gradient of the *j*th coordinate.

#### **III. THE BOUND STATES**

The law of motion of the particles in the bound states depends on the initial conditions (and, consequently, on the value of the energy E), but not on the value of the well depth  $U_0$ . Hence, the forms of distributions and correlation functions of dynamical variables depend on L, but not on u.

For calculation of the distribution functions of dynamical variables in the bound states we shall use the following hypothesis.

*Hypothesis:* For a given value of L the probability to find the system in any part of the surface S is determined by the measure of this part only. This hypothesis comprises three statements. (a) The chaotic component on the surface S is unique; (b) the measure of regular invariant manifolds is equal to zero; (c) the measure of the chaotic component is equal to the measure of the whole surface S.

To check the assumptions (a) and (b) we used  $\varphi - \theta$  maps. The consequent points  $\{\varphi_n, \theta_n\}$ , where  $\varphi_n$  and  $\theta_n$  are the generalized coordinates (see Sec. II) of a chosen particle taken at the moment of its *n*th collision with the billiard wall, were displayed on the two-dimensional plot. At any value of *L* the maps, plotted over  $10^2$  trajectories, were evenly scattered with points without any traces of stability islands, which supports statement (b). The maps, plotted over the only trajectory, looked analogically—the whole maps were scattered evenly—which supports statement (a).

The assumption (c) is an approximation that is asymptotically exact in the limit  $\alpha \rightarrow 0$ , if (a) and (b) hold. The repulsion of particles makes some parts of the surface *S* inaccessible for the system. The measure  $\mu$  of these parts is small together with the parameter  $\alpha$ : if  $L \ll 1$ , then  $\mu \sim \alpha^2$ ; if  $L \rightarrow 1$ , then  $\mu \sim \alpha$ . The hypothesis (c), by neglecting these parts, implies that if W(z) is the distribution function of a dynamical variable *z*, then W(z)dz is the measure of the part of the surface *S* that corresponds to values of this dynamical variable in the interval between *z* and z+dz. In order to find W(z) we have to integrate the Dirac delta function  $\delta(z-z')$  over the induced measure dM, given by Eq. (8).

As an example we present the distribution function W(l) of the angular momentum l of one of the particles for states with given values of L. It is defined by the equality

$$W(l) = \frac{1}{V(L)} \int_{S} \delta(l-l_1) \frac{J}{\sqrt{1-\Phi^2}} dl_1 dp_1 d\theta_1 d\theta_2 d\varphi_1 d\varphi_2,$$
(11)



FIG. 4. The distributions W(l) of the angular momentum of one of the particles for different values of scaled total angular momentum *L*. Continuous lines show the theoretical distributions given by Eq. (13) for values of *L*: (a) 0; (b) 0.2; (c) 0.5; (d) 0.9. The histograms show the numerically found distributions for  $\alpha = 0.3$  (b) and  $\alpha = 0.1$  (c).

$$V(L) = \int_{S} \frac{J}{\sqrt{1-\Phi^2}} dl_1 dp_1 d\theta_1 d\theta_2 d\varphi_1 d\varphi_2.$$
(12)

The sixfold integrals in Eqs. (11) and (12) can be calculated analytically. Thus we obtain

$$W(l) = \frac{8\sqrt{2}\pi^3}{V(L)} \left[1 - |l|\sqrt{2 - 4(L - l)^2} - |L - l|\sqrt{2 - 4l^2}\right]$$
(13)

and

$$V(L) = \frac{8\sqrt{2}\pi^3}{3} \{(4+2L^2)\sqrt{1-L^2} - 6L \ \operatorname{arccos}L + \Theta(1-2L^2)[6L \ \operatorname{arccos}(L\sqrt{2}) - 2(1+L^2)\sqrt{2-4L^2}]\},$$
(14)

where  $\Theta(x)$  is the Heaviside (unit step) function.

The theoretical distributions W(l) for different values of L are shown in Fig. 4 along with the histograms found in the numerical experiment. For each value of L the experimental data were taken from ten trajectories with  $2 \times 10^3$  particle collisions in each. The agreement between theoretical and experimental distributions supports the hypothesis.

The important information about the dynamics of the system can be extracted from the autocorrelation functions of dynamical variables,

$$B_{z}(\tau) = \langle z(t+\tau)z(t) \rangle - \langle z(t) \rangle^{2}, \qquad (15)$$

where z(t) is the value of the variable z at the moment t and the angular brackets denote the averaging over the surface S.

The autocorrelation functions of three variables related to the first particle, namely, its Cartesian coordinate

$$x_1 = \frac{l_1 \cos \varphi_1}{p_1 \sin \theta_1},\tag{16}$$

where V(L) is the volume of the surface S:



FIG. 5. The normalized correlation functions  $b_z(\tau) = B_z(\tau)/B_z(0)$  for different dynamic variables of a particle  $(x, l, and \varepsilon)$  for L=0.3. Each curve has been calculated by averaging over  $10^2$  trajectories of time span  $1.5 \times 10^3$  time units each.

its angular momentum  $l_1$ , and the quantity

$$\varepsilon_1 = p_1^2 - 2l_1^2, \tag{17}$$

which plays the important role in the theory of decay states (see Sec. IV), were calculated numerically for different values of *L*. The ensemble has been formed over  $10^2$  trajectories with length of  $1.5 \times 10^3$  units of time each. The typical forms of autocorrelation functions are shown in Fig. 5.

These forms are too complicated to be exhaustively described by a single parameter. However, we can use the exponential envelope

$$B_{z}^{0}(\tau) = B_{z}(0) \exp\left(-\frac{\tau}{\vartheta_{z}}\right)$$
(18)

to estimate the correlation time  $\vartheta_z$  of the dynamical variable z. Typically the autocorrelation function has the form of dumping oscillations. In this case we find  $\vartheta_z$  and its standard deviation from the best fit of dependence (18) to maxima of absolute values of the autocorrelation function  $|B_z(\tau)|$  in the range  $0 < \tau < 3 \vartheta_z$ . This scheme has been used in Ref. [18]. If  $B_z(\tau)$  decreases monotonically, the formula (18) is used to fit the autocorrelation function itself. The resulting values of  $\vartheta_z$  with their uncertainties are given in the Table I. They are compared to characteristic times of interparticle collisions—the arithmetic mean  $\tau_p = \langle \Delta t_c \rangle$  and the harmonic mean  $\tau'_p = \langle \Delta t_c^{-1} \rangle^{-1}$  of the intervals of time  $\Delta t_c$  between two consequent particles collisions.

TABLE I. Correlation times  $\vartheta$  of dynamical variables  $x_1$ ,  $p_1$ ,  $l_1$ and  $\varepsilon_1 = p_1^2 - 2l_1^2$  and mean times of particles collisions  $\tau_p$  and  $\tau'_p$  at different value of scaled angular momentum *L* for the Bohr biliard with  $\alpha = 0.33$ .

∂\L	0.0	0.3	0.6	0.9
$\vartheta_x$	6.7±0.7	3.6±0.9	11±5	25±4
$\vartheta_p$	$2.8 {\pm} 0.8$	$4\pm1$	$11 \pm 4$	$20 \pm 2$
$\vartheta_{l}$	$7\pm1$	$7\pm2$	12±5	21±7
$\vartheta_{\epsilon}$	$1.4 \pm 0.3$	$2.5 \pm 0.2$	$3.7 \pm 0.7$	88±9
$ au_p$	$2.09 \pm 0.01$	$2.74 \pm 0.01$	$6.50 {\pm} 0.02$	$21.39 \pm 0.04$
$ au_p'$	$0.33 \pm 0.09$	$0.2 \pm 0.1$	$0.17 {\pm} 0.07$	$0.29 {\pm} 0.04$

The value of  $\vartheta_z$  for different quantities z in the range L < 0.5 differs insignificantly and weakly depends on L. For  $L \rightarrow 1$ , on the contrary, the relation  $\vartheta_e \gg \vartheta_p \sim \vartheta_l$  holds. It can be explained by the following reasoning: when the total angular momentum of the system approaches its maximal value, both particles move along the billiard wall colliding almost frontally. Since the masses of the particles are equal, after each collision they interchange their velocities, energies, and angular momenta. The energy and the angular momenta of a particle in these "whispering mode" states are strongly correlated; hence, the change of  $\epsilon$  in each collision turns out to be relatively small, thus leading to longer correlation time.

#### **IV. THE DECAY STATES**

If the parameters of the mechanical state satisfy the inequalities u < 1 and  $L > \sqrt{1-u}$ , then the conservation laws (7) permit the escape of one of the particles to infinity and the Bohr billiard is in a decay state. If after the particle collision the *i*th particle acquires the momentum  $p_i$  and angular momentum  $l_i$  such that

$$\varepsilon_i = p_i^2 - 2l_i^2 > u, \tag{19}$$

then its first collision with the billiard wall will lead to decay.

The process of this "fast" particle having two consecutive collisions with another has small probability. Let  $\kappa = 1$  if one particle collides twice with another without colliding with the billiard wall in between, and  $\kappa = 0$  otherwise. The numerically found value of  $\kappa$  averaged over all particle collisions happens to be negligibly small:  $\langle \kappa \rangle$  never exceeds 3  $\times 10^{-3}$  for u > 1/2.

The surface *S* for the decay states can be divided in two parts: zone *B*, which includes states with particles located within the billiard, and zone *D*, which includes the escape states with at least one particle located outside the billiard. Until the decay occurs, a trajectory does not distinguish from one with the same initial conditions but the other (corresponding to the finite motion) value of the potential depth. So, to analyze the dynamics of the Bohr billiard in zone *B*, which coincides with finite state surface *S*, we may use the finite state measure and the finite state definition of the probability.

If the system stays in zone B long enough for many particle collisions to occur, then we can assume that the distribution of dynamical variables will relax to their equilibrium forms, which have been found in Sec. III for the bound states.

Let us consider the system right after the particles' collision. The probability w of the decay before the next particle collision is equal to

$$w = \frac{1}{V(L)} \int_C \frac{J}{\sqrt{1 - \Phi^2}} dl_1 dp_1 d\theta_1 d\theta_2 d\varphi_1 d\varphi_2. \quad (20)$$

The integration in Eq. (20) is carried over the domain C, that is, the conjunction of those domains  $B_i$  of the zone B where the inequality (20) is fulfilled for the *i*th particle. If L

 $1 \ge \sqrt{1-u}$  or if  $u \ge 1/2$ , then the domains  $B_i$  do not overlap and the integral (19) is equal to

$$w = \frac{2}{V(L)} \int_{B_i} \frac{J}{\sqrt{1 - \Phi^2}} dl_1 dp_1 d\theta_1 d\theta_2 d\varphi_1 d\varphi_2 \quad (21)$$

because of the symmetry with respect to particles interchange. In this formula five integrations out of six could be carried out analytically. The result has the form

$$w = \frac{8\pi^2}{V(L)} \left[ I_1 + 2\Theta(1 - u - 2L^2)I_2 \right], \tag{22}$$

where

$$I_1 = \int_b^c (f_1 - f_2 - f_3) dl_1, \quad I_2 = \int_b^0 (f_2 + f_4) dl_1 \quad (23)$$

and

$$b = \frac{1}{2}(L - \sqrt{1 - u - L^2}), \quad c = \frac{1}{2}(L + \sqrt{1 - u - L^2}).$$
 (24)

The functions  $f_i$  are given by the following expressions:

$$f_1 = \frac{\pi}{2} + \arcsin(1-g), \qquad (25)$$

$$f_2 = l_1 \sqrt{2 - 4(L - l_1)^2} \left[ \frac{\pi}{2} + \arcsin\left( 1 - \frac{1 - 2(L - l_1)^2}{u + 2l_1^2} g \right) \right],$$
(26)

$$f_{3} = (L - l_{1})\sqrt{2 - 4l_{1}^{2}} \left[\frac{\pi}{2} + \arcsin\left(1 - \frac{2(L - l_{1})^{2}}{1 - u - 2l_{1}^{2}}g\right)\right],$$
(27)

$$f_{4} = l_{1}\sqrt{2 - 4(L - l_{1})^{2}} \times \left[\frac{\pi}{2} + \arcsin\left(1 - \frac{2l_{1}^{2}}{1 - u - 2(L - l_{1})^{2}}g\right)\right], \quad (28)$$

where

$$g = \frac{2u}{1 - 2l_1^2 - 2(L - l_1)^2}.$$
 (29)

The most stable states correspond to the case when quantities  $\xi = 1 - u$  and  $\eta = \sqrt{1 - u} - L$  tend to zero. In this case w vanishes no slower than  $\xi^{1/2} \eta^{1/4}$ .

If after the given collision the condition of the decay (19) is not fulfilled for any particle, then the escape may become possible only after the next particle collision. We assume that the particle collision transfers the system to any state in S with equal probability. For the states with  $w \ll 1$  this assumption yields the exponential decay law: the probability P(t) for the system to stay in zone B for the time t is

$$P(t) = e^{-\gamma t}.$$
 (30)

The decay rate  $\gamma$  is given by the ratio of the probability of decay in a given state w to the average time  $\tau_p$  between two consequent particles collision:

$$\gamma(u,L,\alpha) = \frac{w(u,L)}{\tau_p(L,\alpha)}.$$
(31)

The value of  $\tau_p$  can be basically borrowed from the model of the hard-sphere gas as the average time of free flight (see, e.g., Ref. [19]):

$$\tau_p \approx \frac{1}{n \, \sigma v},\tag{32}$$

where *n* is the concentration of particles,  $\sigma$  is the scattering cross section, and *v* is the averaged relative velocity of the colliding particles. For the Bohr billiard we can take

$$n = \frac{2}{\pi}, \quad \sigma = 4\alpha, \quad v = 1. \tag{33}$$

Thus we obtain the estimate

$$\tau_p = \frac{\pi}{8\,\alpha}.\tag{34}$$

This approximation must be improved by account of the dependence of  $\tau_p$  on L, which is essential in the range  $L > L_b$ , where both particles have the components of the angular momenta of the same sign. It is easy to visualize the limit  $L \rightarrow 1$ , when both particles move along the "whispering mode" trajectories in the same direction with nearly the same velocities. Thus we can expect that both concentration n and relative velocity v appear to be L dependent.

At first we consider the influence of *L* on the concentration *n*. For  $L > L_b$  the particles are located between the billiard wall and the concentric circle with radius  $\rho = \sqrt{2L^2 - 1}$ . Then for this range of *L* we must exclude the inaccessible area  $\Sigma' = \pi \rho^2$  from the billiard area  $\Sigma = \pi$ . Thus we obtain the following expression for the concentration of particles:

$$n_1 = \frac{1}{\pi(1 - L^2)}.$$
 (35)

For the extremely large values of  $L \ge \sqrt{1-2\alpha+2\alpha^2}$ , when  $\rho \ge 1-2\alpha$ , the motion of particles is essentially one dimensional in the narrow ring along the billiard wall. In this case the concentration is given by the equality

$$n_2 = \frac{1}{2\pi(\alpha - \alpha^2)}.$$
(36)

Secondly, for  $L \rightarrow 1$  the average relative velocity of the particles tends to zero as  $v \sim \sqrt{1-L^2}$ . One can take for the range  $L > L_b$  the approximation

$$v = \sqrt{2 - 2L^2}.\tag{37}$$

This formula has correct asymptotics at  $L \rightarrow 1$  and matches with the low-*L* value v = 1 at  $L = L_b$ .

From Eqs. (32) and (33) and (35) and (37) we finally obtain the three-piecewise expression for the time of interparticle collisions:

$$\tau_p = \frac{\pi}{4\sqrt{2}\alpha} \sqrt{1-L^2}, \quad \frac{1}{\sqrt{2}} < L < \sqrt{1-2\alpha+2\alpha^2}, \quad (38)$$
$$\pi = 1-\alpha$$

$$\tau_p = \frac{\pi}{2\sqrt{2}\alpha} \frac{1-\alpha}{\sqrt{1-L^2}}, \quad \sqrt{1-2\alpha+2\alpha^2} < L < 1.$$

These formulas match at the interval borders.

#### V. NUMERICAL STUDY OF DECAY

For the numerical study of the process of decay in the Bohr billiard the ensemble of initial conditions that is uniform on the surface S has been prepared by the following procedure. The distribution of the Cartesian components of momenta has been created uniform on the surface of the four-dimensional hypersphere  $\mathbf{p}_1^2 + \mathbf{p}_2^2 = 1$ , which corresponds to the states with energy E = 1/2. To do this we have first created with the standard generator of the random numbers the uniform momenta distribution within a square of size equal to 2. Then we have excluded all points out of the required sphere. The last step was the renormalization of momenta to make all the remaining points lie on the surface  $\mathbf{p}_1^2 + \mathbf{p}_2^2 = 1$ . The distribution of initial values of Cartesian coordinates of particles has been created uniform within the well (in a way similar to that in the case of momenta); then the points with  $r_{12} \leq 2\alpha$  were excluded. From these distributions the subset of initial conditions that correspond to the states with a prescribed value of scaled angular momentum L within a given error limit ( $\Delta L = 5 \times 10^{-3}$ ) has been selected.

For a given set of initial conditions the equations of motion were integrated forward and backward in time until the moments of decay ( $t_+$  and  $t_-$ , respectively), when one of the particles left the well. The sum  $t_d = t_+ + t_-$  gives the delay time of the state. The integration has been interrupted if no decay occurred before the cutoff time  $t_c$ . The usual value of  $t_c$  was 10<sup>4</sup>, but in the case of low energy and high angular momentum we needed to take  $t_c$  equal to  $5 \times 10^4$ . For each set of u and L the number of trajectories was 10<sup>4</sup>.

Values of  $\gamma$  have been estimated from the decay law (30) at the moments when P(t) = 2/3 and 1/3 for both directions of time.

Additional values of  $\gamma$  were found from the distribution of delay times. If the decay can be described by the exponential law (30) and the times of direct and inverse decays  $t_+$  and  $t_-$  are independent, then the distribution of delay times  $t_d$  has the form

$$W(t_d) = \gamma^2 t_d \exp(-\gamma t_d). \tag{39}$$

The experimental value of  $\gamma$  was determined from the best fit of the theoretical distribution (39) to the experimental one  $W_e(t_d)$ . The minimal value of the deviation

$$\delta_W(\gamma) = \int_0^{2t_c} W_e(t_d) - W_e(t_d) \big| dt_d \tag{40}$$



FIG. 6. The dependence of decay rate  $\gamma$  on energy variable u and the scaled angular momentum L for the Bohr billiard with  $\alpha = 0.3$  in a semilogarithmic scale. Continuous lines show the theoretical values given by formula (38) for values of u: (a) 0.99; (b) 0.95; (c) 0.91; (d) 0.67. Experimental data are plotted by dots. Dashed vertical lines mark the limiting values of L for the decay states.

gives the estimate of the accuracy of the exponential law of decay. Values of  $\delta_W$  lie usually in the range  $\delta_W < 0.1$ . For large *L*, when the number of experimental points is small, the fluctuations of the experimental delay time distribution raise values of  $\delta_W$  as high as 0.5. Nevertheless, in these cases the approximation remains acceptable since the theoretical curve lies within the standard deviation bands of the histograms.

The values of  $\gamma$  for given u and L, which are found by different procedures, can be described by the mean value  $\overline{\gamma}$  and the standard deviation  $\Delta \gamma$ . The relative error  $\delta_{\gamma} = \Delta \gamma / \overline{\gamma}$  does not exceed  $10^{-2}$  for u = 0.99 and increases to  $\delta_{\gamma} = 0.2$  for u = 0.67.

### VI. DISCUSSION

Above we have presented a theory of the decay process in the Bohr billiard. It is based on the assumptions of the exponentiality of the decay [Eq. (30)] and uses the stationary distributions of dynamical variables in the transient case. This approach is valid for relatively small decay rate, when  $\gamma \tau_p \ll 1$ . Theoretical dependence  $\gamma(u)$  is shown in Fig. 6 for different values of *L*. The numerically found values of  $\gamma$  are plotted on the same figure by dots. The error bars are comparable to the size of a dot for all points but one. The level of agreement can be considered satisfactory for a theory without any adjustable parameters if one takes into account that in the studied domain of parameters  $\gamma$  varies over nearly 4 orders of magnitude.

The dependence of decay rate on *L* is essential even for small and medium values of total angular momentum: the ratio of rates of the decay taken at L=0 and  $L=0.7\sqrt{1-u}$  is about 10 for all considered values of *u*. For the states with u < 1/2 the two-particle decay is possible, and the assumption  $w \ll 1$ , crucial for the exponential law, does not hold. Nearly all states in this range decay after a few times of free passage; only in the range  $L \approx \sqrt{1-u}$  can one find trajectories with many particle collisions.

A novel feature unveiled by the numerical experiment is the presence of the long-living states for which the times  $t_{+}$ or  $t_{-}$ , but not both of them, exceed the cut-off time  $t_{c}$ . The existence of these states leads to the suggestion that the decay law at large t has the power behavior  $P(t) \sim t^{-v}$ . This type of decay law is known in the theory of transient chaos [15]. It originates from the presence of the domain of nondecaying states that has finite measure. Sticking of the trajectories in the vicinity of KAM surfaces enclosing this domain give rise to long-living decay states [20,21]. Alternatively, these states may indicate the possibility of the capture of incoming particles in the Bohr billiard. The rigorous proof of the existence of stable states with finite  $t_{-}$  and infinite  $t_{+}$  (or vice versa) could not be given either by numerical means or by approximate approaches. We leave this problem for future investigations.

In our studies we have used the ensemble of the initial conditions, in which they are spread uniformly in the zone B of the phase surface S. This uniform ensemble can be characterized by two parameters u and L; it is convenient for

studying transient chaos. The original Bohr's problem is connected to the ensemble of a different type, the scattering ensemble. It can be characterized by two parameters, namely, the energies  $E_1$  and  $E_2$  of the particles in the instate, when the incoming particle 1 is located outside the billiard. The other parameters of the state (the impact parameter of the particle 1, the coordinates of the particle 2, and the angle  $\theta_2$ ) in the scattering ensemble are distributed uniformly. The distribution of the delay times for the scattering ensemble differs essentially from that given by Eq. (30). The overwhelming contribution in the range of small  $t_d$  comes from the passage trajectories without any interparticle collisions. The medium  $t_d$  range can be described by the appropriate integration of the distribution (38) weighted with the distribution of L in the scattering ensemble.

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