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Quantum chaos for the radially vibrating spherical billiard

Richard L. Liboff and Mason A. Porter
Schools of Electrical Engineering and Applied Physics and Center for Applied Mathematics, Cornell University, Ithaca, New York 14853

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The spherical quantum billiard with a time-varying radius, $a(t)$, is considered. It is proved that only superposition states with components of common rotational symmetry give rise to chaos. Examples of both nonchaotic and chaotic states are described. In both cases, a Hamiltonian is derived in which a and P are canonical coordinate and momentum, respectively. For the chaotic case, working in Bloch variables (x,y,z), equations describing the motion are derived. A potential function is introduced which gives bounded motion of $a(t)$. Poincaré maps of (a,P) at $x=0$ and the Bloch sphere projected onto the (x,y) plane at $P=0$ both reveal chaotic characteristics. © *2000 American Institute of Physics.* [S1054-1500(00)00602-9]

Quantum billiards describe the motion of a point particle undergoing perfectly elastic collisions inside a domain with a closed boundary. In the present paper, we consider the spherical quantum billiard with a radially vibrating surface. Quantum chaos can occur in this case if one considers the superposition of at least two eigenstates. The manifestation of this behavior depends on the relative quantum numbers of the two superposed eigenstates. These results are of both theoretical and practical interest. On the theoretical side, they motivate the definition of the degree-of-vibration of a quantum billiard with a time-dependent boundary and set the stage for a new class of quantum chaos. On the practical side, the radially vibrating spherical quantum billiard can be considered as a model for particle behavior in the nucleus as well as a model of the quantum-dot microdevice component.

I. INTRODUCTION

Quantum chaos has been studied extensively in the recent past.[1–5] Quantum chaotic properties of a particle confined to a one-dimensional box with vibrating walls is well established.[6] In the present work, we consider the spherical quantum billiard with a time-varying boundary which is in a superposition state of two eigenstates of the system. A theorem is derived that only superposition states with components of common rotational symmetry give rise to chaos. An example of the nonchaotic case is given in terms of a superposition state of the two azimuthally symmetric eigenfunctions of lowest energy. The theorem is then proved for an arbitrary superposition state. In this proof, nonchaotic behavior is established by showing that equations reduce to autonomous equations in two dimensions, whose nonchaotic properties are well known.[7] An example is then presented of a chaotic two-component superposition state, in which Bloch variables are brought into play.[8–10] A Hamiltonian is derived in which a and P are canonical coordinate and momentum, respectively. A potential function is introduced which implies bounded motion of the spherical radius $a(t)$. Poincaré maps of (a,P) at a fixed value of one of the Bloch variables and the projection of the Bloch sphere onto the (x,y) plane at $P=0$ both reveal chaotic characteristics. Corresponding to a slight change in initial conditions, structure in related plots indicates that for this new initial data, not all invariant tori are destroyed in the configuration in accord with KAM theory. A discussion is included on the corresponding chaotic behavior of the vibrating spherical classical billiard. It is noted that the radially vibrating quantum billiard has application as a model for intradynamics of the nucleus[11] and the ''quantum dot.''[12] At low temperature this latter microdevice component experiences vibrations due to zero-point motions. At higher temperatures, it exhibits vibrations due to natural fluctuations. Additionally, the ''liquid drop'' and ''collective'' models of the nucleus include boundary vibrations. A degree of vibration of a system is characterized by a time-dependent displacement parameter of the system. For example, a rectangle in the plane with moveable boundaries has two degrees of vibration.

II. NONCHAOTIC CONFIGURATION

The spherical quantum billiard refers to the quantum dynamics of a particle of mass m confined to the interior of a spherical cavity of mass $M \gg m$, with smooth walls of radius a. In the present configuration, $a=a(t)$. A two-component superposition state of this quantum billiard is given by

$$|\psi(r,\theta,\phi,t)\rangle = A_1(t)|lnm,t\rangle + A_2(t)|l'n'm',t\rangle, \tag{1a}$$

where $A_1(t)$ and $A_1(t)$ are complex amplitudes. The numbers (l,n,m) are orbital, principal, and azimuthal quantum numbers, respectively, and eigenstates are products of spherical Bessel functions and spherical harmonics.[13] In the coordinate representation,

$$\langle \mathbf{r}|lnm,t\rangle = \psi_{lnm}(r,\theta,\phi,t) = \sqrt{\frac{2}{a^3(t)}}\left(\frac{1}{j_{l+1}(x_{ln})}\right) \times j_l\left(\frac{r x_{ln}}{a(t)}\right) Y_{lm}(\theta,\phi), \tag{1b}$$

$$j_l(x_{ln}) = 0. \tag{1c}$$

It is shown that the condition of common rotational symmetry of the two eigenstates in (1a),

$$l=l', \quad m=m', \tag{1d}$$

is necessary for chaotic behavior of this superposition state. The explicit time dependence of eigenstates is in their normalization factors as well as in arguments of spherical Bessel function components [see (1b)]. First, we present an example to motivate the preceding theorem. In the following section, the theorem is proved for an arbitrary superposition state. An example is then given of a superposition state that exhibits chaotic behavior.

The time-dependent Schrödinger equation for the system at hand is given by

$$i\hbar \frac{\partial \psi(r,\theta,\phi,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi(r,\theta,\phi,t) \tag{1e}$$

for $r<a(t)$. Taking expectations of this equation in the superposition state (1a) gives

$$\left\langle \psi \middle| \left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi\right\rangle = \frac{1}{a^2}[\varepsilon_1|A_1|^2+\varepsilon_2|A_2|^2] \equiv K(A_1,A_2,a), \tag{2a}$$

$$i\hbar\left\langle \psi \middle| \frac{\partial\psi}{\partial t}\right\rangle = \dot{A}_1A_1^*+\dot{A}_2A_2^*+\mu|A_1|^2+\sigma|A_2|^2+\gamma A_1A_2^* + \lambda A_2A_1^* \tag{2b}$$

$$\varepsilon_1 \equiv \frac{\hbar^2 x_{ln}^2}{2m}, \quad \varepsilon_2 \equiv \frac{\hbar^2 x_{l'n'}^2}{2m}. \tag{2c}$$

The diagonal form of the expectation of the Laplacian follows from spherical Bessel-function orthogonality. This orthogonality does not carry over to the expectation of the time derivative, as this operation causes r-dependent terms to appear in the integrand due to differentiation of $a(t)$ in the argument of the spherical Bessel function (1b). Examining the superposition of $|010\rangle$ and $|110\rangle$, with (2b) and orthogonality of spherical harmonics, one obtains

$$\mu=\sigma=\gamma=\lambda=0. \tag{2d}$$

Equating (2a) and (2b) gives

$$i\dot{A}_1 = \frac{1}{\hbar a^2}\varepsilon_1 A_1, \quad i\dot{A}_2 = \frac{1}{\hbar a^2}\varepsilon_2 A_2, \tag{2e}$$

where $\varepsilon_1,\varepsilon_2$ are given by (2c).

These latter equations may be integrated to yield

$$A_1(t) = C_1 \exp\left[-\frac{i\varepsilon_1}{\hbar}\int a^{-2}(t)\,dt\right],$$

$$A_2(t) = C_2 \exp\left[-\frac{i\varepsilon_2}{\hbar}\int a^{-2}(t)\,dt\right]. \tag{3a}$$

One may construct a classical Hamiltonian corresponding to the motion (2d). Namely, with (2a) one obtains

$$H=\frac{P^2}{2M}+K(A_1,A_2,a)+V(a) = \frac{P^2}{2M}+\frac{1}{a^2}[\varepsilon_1\alpha+\varepsilon_2\beta]+V(a), \tag{3b}$$

where with (3a),

$$\alpha \equiv |A_1|^2 = |C_1|^2, \tag{3c}$$

$$\beta \equiv |A_2|^2 = |C_2|^2. \tag{3d}$$

Hamilton's equation for da/dt gives

$$\dot{a} = \frac{P}{M}. \tag{3e}$$

In the preceding equation, $V(a)$ is an arbitrary potential and $M \gg m$ is the effective mass of the spherical enclosure. As is well known, a Hamiltonian with no explicit time dependence and one degree-of-freedom corresponds to a two-dimensional autonomous system, which is known to be nonchaotic.[14]

III. NECESSARY CONDITIONS FOR CHAOS IN K COUPLED STATES

Consider the general superposition state relevant to a system

$$\psi = A_1\varphi_{q_1}+A_2\varphi_{q_2}+\cdots+A_k\varphi_{q_k}, \tag{4a}$$

where $q_i \equiv (l_i,n_i,m_i)$. If there does not exist a pair of eigenfunctions in the sum (5a) that have common angular quantum numbers [i.e., there is no pair, (i,i') such that $(l_i = l_{i'},\ m_i=m_{i'})$], then forming the norm of (4a) returns a diagonal form

$$\dot{A}_1A_1^*+\cdots+\dot{A}_kA_k^* = \delta_1|A_1|^2+\cdots+\delta_k|A_k|^2. \tag{4b}$$

All the cross terms vanish by orthogonality of spherical harmonics. The diagonal terms stem from the Laplacian. Following the procedure above gives the Hamiltonian $H = H(a,P)$:

$$H=\frac{P^2}{2M}+\frac{1}{a^2}\sum_{i=1}^{k}\varepsilon_i\alpha_i+V(a), \quad \alpha_i \equiv |A_i|^2=|C_i|^2; \tag{4c}$$

$$\sum_{i=1}^{k}|C_i|^2=1, \quad C_i=\text{constant}. \tag{4d}$$

The superposition (4a) is nonchaotic because the Hamiltonian is again autonomous with one degree-of-freedom.

We may conclude that a necessary condition for chaotic behavior of an arbitrary superposition state for a system is that at least one pair of functions in the expansion have common angular quantum numbers. Note, for example, that coupling exists between the states

$$J_l\left(\frac{rx_{ln}}{a}\right)Y_{lm}(\theta,\phi), \quad j_l\left(\frac{rx_{ln'}}{a}\right)Y_{lm}(\theta,\phi), \tag{4e}$$

a superposition of which, in general, leads to chaos. In particular, considering small (n,n'), we may obtain a chaotic superposition for eigenstates with small energies. That is, we need not consider only the high quantum number limit in order to obtain chaotic behavior, as is the case in most studies of quantum chaos.[1,4] Note also that this proof applies equally for a radially vibrating cylindrical quantum billiard of fixed length in which spherical Bessel functions are replaced by Bessel functions of the first kind, and spherical harmonics are replaced by elementary harmonic functions.

IV. CHAOTIC CONFIGURATION

As an example of a chaotic configuration, consider the azimuthally symmetric superposition state

$$|\psi(l,n,m)\rangle = A_1|110\rangle + A_2|120\rangle. \tag{5a}$$

Denoting the expectations of the left and right sides of (1e) by T and K, respectively, one obtains

$$T = \mu\frac{\dot{a}}{a(t)}[-A_1^*A_2 + A_1A_2^*] + \dot{A}_1A_1^* + \dot{A}_2A_2^*, \tag{5b}$$

$$\mu \simeq 0.4395263. \tag{5c}$$

(The parameter μ may be expressed analytically but takes up far too much space and is unsightful.) Again the momentum equation (3e) and the Hamiltonian (3b) apply. Combining (5b) with (2a) and noting that A_1^* and A_2^* may be taken as independent parameters [or, equivalently, treating (5b) as a quadratic form] gives the matrix equation

$$i\dot{A}_n = \sum_{n=1}^{2} D_{nk}A_k, \tag{5d}$$

where D is the Hermitian matrix

$$D = \begin{pmatrix} \varepsilon_1/\hbar a^2 & -i\mu\dot{a}/a \\ i\mu\dot{a}/a & \varepsilon_2/\hbar a^2 \end{pmatrix}, \tag{5e}$$

$$\varepsilon_1 \equiv \frac{\hbar^2 x_{11}^2}{2m}, \quad \varepsilon_2 \equiv \frac{\hbar^2 x_{12}^2}{2m} > \varepsilon_1, \tag{5f}$$

and μ is given by (5c).

Introducing the Bloch variables[8–10]

$$x = A_1A_2^* + A_2A_1^*, \quad y = i(A_1^*A_2 - A_1A_2^*),$$
$$z = A_2A_2^* - A_1A_1^* = |A_2|^2 - |A_1|^2 \tag{6a}$$

gives, with (5d) and (5e),

$$\dot{x} = -\omega_0 y/a^2 - 2\mu Pz/Ma,$$
$$\dot{y} = \omega_0 x/a^2,$$
$$\dot{z} = 2\mu Px/Ma,$$
$$\hbar\omega_0 \equiv (\varepsilon_2 - \varepsilon_1). \tag{6b}$$

Rewriting $K(A_1,A_1,a)$ in terms of the Bloch variable z gives

$$K(z,a) = (\varepsilon_+ + z\varepsilon_-)/a^2,$$
$$\varepsilon_\pm \equiv (\varepsilon_2 \pm \varepsilon_1)/2. \tag{6c}$$

Inserting $K(z,a)$ into (3b) gives Hamilton's equations

$$\dot{a} = P/M,$$
$$\dot{P} = -\frac{\partial V}{\partial a} + 2[\varepsilon_+ + \varepsilon_-(z - \mu x)]/a^3. \tag{6d}$$

Equations (6b) and (6d) are a set of five coupled equations for our system. The constants of motion for this system are the radius of the Bloch sphere

$$x^2 + y^2 + z^2 = 1 \tag{7a}$$

and the energy

$$E = P^2/2M + V(a) + K(z,a), \tag{7b}$$

so that there remain three independent dynamical variables. The system of equations (6b) and (6d) are a full set of dynamical equations for the variables (x,y,z,a,P) whose equilibrium points satisfy $x=0$, $y=0$, $z=\pm 1$, $a=a_\pm$, $P=0$, where $a_\pm$ are solutions to the second equation in (6d) for $x = P = 0$ and $z=\pm 1$. Providing $V(a)+K(z,a)$ has a single minimum in a, these fixed points are stable elliptic. (That is, every eigenvalue of the Jacobian of the linearized system is purely imaginary. For the system at hand, there is only one zero eigenvalue and two pairs of purely imaginary conjugate eigenvalues.)

Oscillation of the radius $a(t)$ in a bounded radial interval is implied by the total potential

$$V_0(a-a_0)^2/a_0^2 + (\varepsilon_+ + z\varepsilon_-)/a^2 \tag{8a}$$

for which $a_\pm$ are given by solutions of the equation

$$a - a_0 = a_0^2\varepsilon_\pm/V_0a^3. \tag{8b}$$

A single real solution of (8b) corresponds to each of the $\varepsilon_\pm$ values which, as noted previously, are both positive. One finds that

$$a_+ > a_- > a_0. \tag{8c}$$

It follows that if $a_- \leqslant a(0) \leqslant a_+$, $a(t)$ likewise remains bounded in the interval $[a_-, a_+]$. It is noted that the analysis of this last section parallels the one-dimensional study of Blümel and Esser.[3]

Poincaré maps of (a,P) at $x=0$ are shown in Figs. 1(a) and 1(b) and that of the Bloch spheres projected onto the (x,y) plane at $P=0$ are shown in Figs. 2(a) and 2(b). These maps illustrate the chaotic behavior of the spherical quantum billiard with a vibrating surface. Working in units of $\hbar = 1$, data and initial values used in calculations of Figs. 1(a) and 2(a) are as follows: $x(0) = \sin 0.95\pi$, $y(0)=0$, $z(0) = \cos 0.95\pi$, $a_0 = 1.25$, $a(0) \simeq 0.504967$, $P(0)=0$, $M=10$, $\varepsilon_1 \simeq 10.09536$, $\varepsilon_2 \simeq 29.83967$, $\mu \simeq 0.439526$, and $V_0/a_0^2 = 5$. We now make a slight change in starting data. Namely, with all data the same, except for $a(0)=0.75$ and $P(0)=2.5$, related Poincaré maps are shown in Figs. 1(b) and 2(b). The additional structure in these graphs indicate that corresponding to a slight change in initial data, not all of the invariant tori of the given dynamical configuration are broken up, which is in accord with KAM theory.

As quantum chaos has been established for the present system, it is natural to ask about the nature of the corresponding chaotic behavior in real space. For the stationary spherical classical billiard, due to conservation of angular

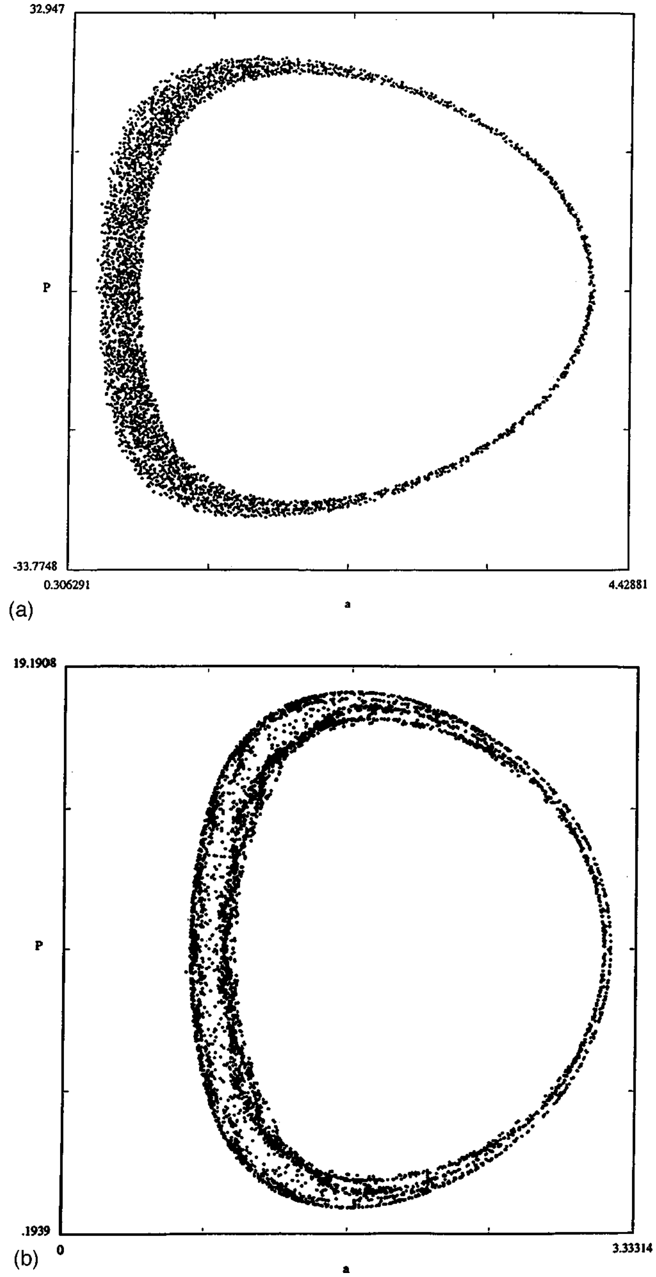

FIG. 1. (a) Poincaré map of (a,P) at $x=0$. (b) Same Poincaré map as in (a), illustrating that for the varied initial conditions, $[a(0)=0.75,\ P(0)=2.5)]$ invariant tori have not all been destroyed.

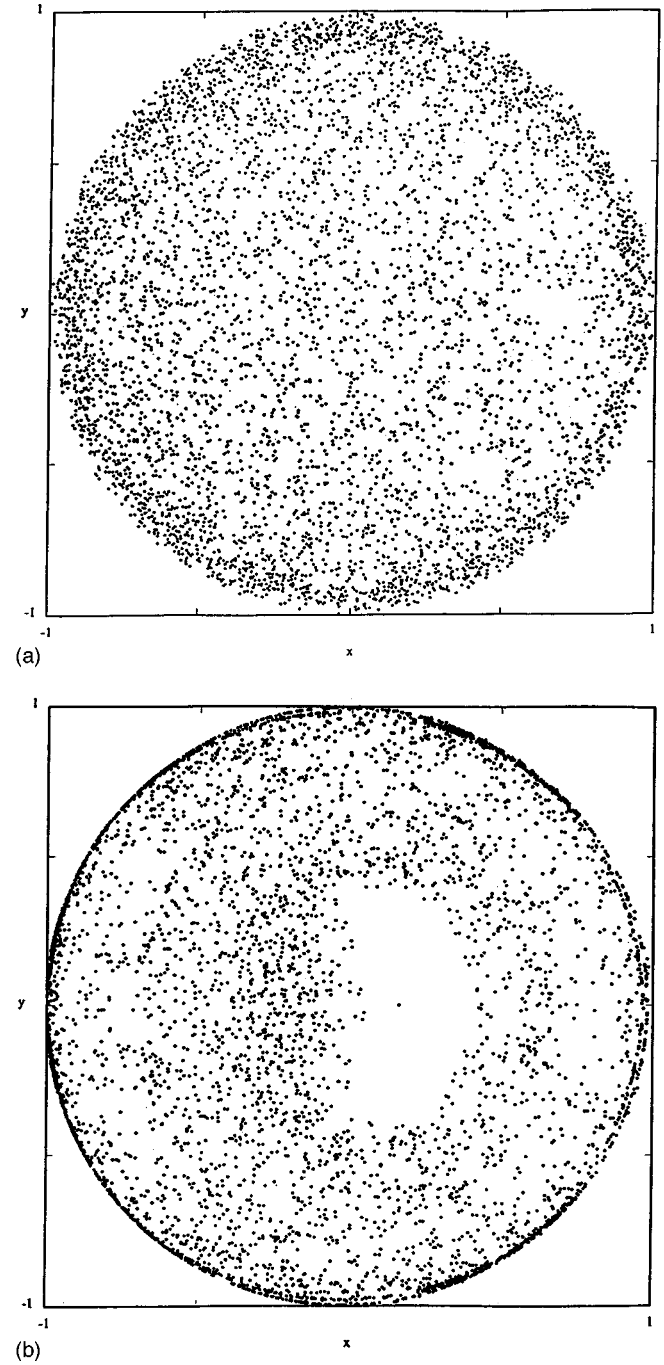

FIG. 2. (a) Poincaré map of the Bloch sphere projected onto the (x,y) plane at $P=0$. (b) Same Poincaré map as in (a), illustrating that for the varied initial conditions, $[a(0)=0.75,\ P(0)=2.5)]$ invariant tori have not all been destroyed.

momentum, the particle trajectory sweeps out an annular domain of constant inner radius.[15] Vibration of the wall of the sphere destroys this constant and chaotic motion may be expected to develop. (The ''moment arm'' of the reflected trajectory increases during, say, the expansion phase of the sphere.) In addition, we consider the following connection between classical and quantum chaos is the present context. As a mathematical abstraction (6a) and (6b) may also be viewed as classical equations of motion for the five given variables which give rise to Hamiltonian chaos. The quantum interpretation of these dynamics may be seen in two manners. First, the Bloch variables x,y,z correspond to the quantum probabilities $|A_1|^2, |A_2|^2$. Second, quantum mechanical wave functions of the given system depend on these variables.

V. CONCLUSIONS

The spherical quantum billiard with a time-varying boundary was studied. It was shown that an arbitrary superposition state of a system is chaotic provided that at least two components of the superposition state have common rotational symmetry. Examples of both nonchaotic and chaotic states were described. For the chaotic case, working in Bloch variables, a Hamiltonian was derived in which the spherical radius is a canonical coordinate. A potential function was introduced which leads to bounded motion of the spherical radius. Two sets of Poincaré maps were observed to reveal chaotic characteristics. A discussion was included on the corresponding chaotic behavior of the classical vibrating spherical billiard.

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