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VIBRATING QUANTUM BILLIARDS ON RIEMANNIAN MANIFOLDS

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Quantum billiards provide an excellent forum for the analysis of quantum chaos. Toward this end, we consider quantum billiards with time-varying surfaces, which provide an important example of quantum chaos that does not require the semiclassical ($\hbar \to 0$) or high quantum-number limits. We analyze vibrating quantum billiards using the framework of Riemannian geometry. First, we derive a theorem detailing necessary conditions for the existence of chaos in vibrating quantum billiards on Riemannian manifolds. Numerical observations suggest that these conditions are also sufficient. We prove the aforementioned theorem in full generality for one degree-of-freedom boundary vibrations and briefly discuss a generalization to billiards with two or more degrees-of-vibrations. The requisite conditions are direct consequences of the separability of the Helmholtz equation in a given orthogonal coordinate frame, and they arise from orthogonality relations satisfied by solutions of the Helmholtz equation. We then state and prove a second theorem that provides a general form for the coupled ordinary differential equations that describe quantum billiards with one degree-of-vibration boundaries. This set of equations may be used to illustrate KAM theory and also provides a simple example of semi-quantum chaos. Moreover, vibrating quantum billiards may be used as models for quantum-well nanostructures, so this study has both theoretical and practical applications.

1. Introduction

The study of quantum billiards encompasses an essential subdiscipline of applied dynamics. Within this field, the search for chaotic behavior is one component of a large segment of literature concerning quantum chaos [Gutzwiller, 1990; Casati, 1985; Casati & Chirikov, 1995]. The radially vibrating spherical billiard, for example, may be used as a model for particle behavior in the nucleus [Wong, 1990] as well as for the quantum dot microdevice component [Lucan, 1998]. Additionally, the vibrating cylindrical quantum billiard may be used as a model for the quantum wire, another microdevice. Other geometries of vibrating quantum billiards have similar applications. Moreover, vibrating quantum billiards may be used to model Fermi accelerators [Badrinarayanan & José, 1995; Lichtenberg & Lieberman, 1992], which provide a description of cosmic ray acceleration. The study of quantum chaos in vibrating quantum billiards is thus important both because it expands the mathematical theory of dynamical systems and because it can be applied to problems in mesoscopic physics.

Quantum billiards have been studied extensively in recent years [Blümel & Esser, 1994; Gutzwiller, 1990; Casati, 1985; Casati & Chirikov, 1995]. These systems describe the motion of a point particle undergoing perfectly elastic collisions in a bounded domain with Dirichlet boundary conditions. Blümel and Esser [1994] found quantum chaos in the linear vibrating quantum billiard. Liboff and Porter [2000] extended these results to spherical quantum billiards with

vibrating surfaces and derived necessary conditions for these systems to exhibit chaotic behavior. One of the primary goals of this paper is to generalize these results to other geometries.

In the present work, we derive necessary conditions for the existence of chaos in vibrating quantum billiards on Riemannian manifolds. We prove such a result in full generality for one degree-of-freedom boundary vibrations (henceforth termed *degree-of-vibration* (*dov*)) and also briefly discuss a generalization to quantum billiards with two or more *dov*. In the "vibrating quantum billiard problem," the boundaries of the billiard are permitted to vary with time. The *degree-of-vibration* of the billiard describes the number of independent boundary components that vary with time. If the boundary of the billiard is stationary, it is said to have zero *dov*. The radially vibrating sphere and the linear vibrating billiard each have one *dov*. The rectangular quantum billiard in which both the length and width are time-dependent has two *dov*.

The requisite conditions for chaotic behavior in one *dov* billiards are direct consequences of the separability of the Helmholtz equation [Liboff, 1999] in a given orthogonal coordinate frame, and they arise from orthogonality relations satisfied by solutions of the Helmholtz equation. We also state and prove a second theorem that gives a general form for the coupled ordinary differential equations that describe quantum billiards with one *dov*. These equations provide an illustration of KAM theory, so they are important for both research and expository pursuits.

2. Quantum Billiards with One Degree-of-Vibration

Quantum billiards describe the motion of a point particle of mass m_0 undergoing perfectly elastic collisions in a domain in a potential V with a boundary of mass $M \gg m_0$. (Though m_0/M is small, we do not pass to the limit in which this ratio vanishes.) With this condition on the mass ratio, we assume that the boundary does not recoil from collisions with the point particle confined therein. Point particles in quantum billiards possess wavefunctions that satisfy the Shrödinger equation, whose time-independent part is the Helmholtz equation. Globally separable quantum billiards with "stationary" (i.e. zero *dov*) boundaries exhibit only integrable behavior. That is, the motion of their associated wavefunctions may only be periodic and quasiperiodic. Two types of quantum billiard systems in which this global separability assumption is violated are ones with concave boundary components and ones with composite geometry. Both of these situations exhibit so-called "quantized chaos" (or "quantum chaology") [Gutzwiller, 1990; Blümel & Reinhardt, 1997]. Perhaps the best-known example of a geometrically composite quantum billiard is the stadium billiard [Katok & Hasselblatt, 1995; Arnold, 1988; MacDonald & Kaufman, 1988] which consists of two semicircles connected by lines to form a "stadium." In the present paper, we retain the assumption of global separability but permit the boundaries of the quantum billiards to vary with time.

2.1. *Necessary conditions for chaos*

In [Liboff & Porter, 2000], it was shown that any k-superposition state of the radially vibrating spherical quantum billiard must include a pair of eigenstates with rotational symmetry (in other words, with equal orbital (l) and azimuthal (m) quantum numbers) in order for the superposition to exhibit chaotic behavior. One of the goals of the present paper is to prove the following generalization:

Theorem 1. *Let X be an s-dimensional Riemannian manifold with (Riemannian) metric g. Assume the Helmholtz operator $T \equiv \nabla^2 + \lambda^2$ is globally separable on (X, g), so that one may write the wave-function ψ as the superposition*

$$\psi(x) = \sum_n \alpha_n(t) A_n(t) \psi_n(x)\,, \tag{1}$$

where $x \equiv (x_1, \ldots, x_s)$ is the position vector, $n \equiv (n_1, \ldots, n_s)$ is a vector of quantum numbers, and

$$\psi_n(x) = \prod_{j=1}^{s} f_j^{(n_j)}(x_j) \tag{2}$$

is a product of s "component functions" $f_j^{(n_j)}(x_j)$. The parameter α_n is a normalization constant, and $A_n(t)$ is a complex amplitude. If the quantum billiard of boundary mass M defined on (X, g) experiences one dov in a potential $V = V(a)$, where a describes the time-dependent dimension of the boundary, then for any k-term superposition state to manifest chaotic behavior, it is necessary that there exist a pair among the k states whose $s - 1$

quantum numbers not corresponding to the vibrating dimension are pairwise equal. (*That is, for some pair of eigenstates with respective quantum numbers* $(n_{k_1}, \ldots, n_{k_{s-1}})$ *and* $(n'_{k_1}, \ldots, n'_{k_{s-1}})$ *corresponding to nonvibrating dimensions, one must have* $n_{k_j} = n'_{k_j}$ *for all* $j \in \{1, \ldots, s-1\}$.)

In other words, the above theorem states that given a globally separable vibrating billiard, a superposition state of a one *dov* quantum billiard whose geometry is described by an s-dimensional orthogonal coordinate system must have a pair of eigenstates with $(s-1)$ equal quantum numbers corresponding to the stationary dimensions of the billiard's boundary in order to exhibit chaotic behavior. For a discussion of the separability of the Helmholz operator, see Appendix A. Examples of manifolds on which this operator is globally separable include well-known ones such as rectangular, cylindrical (polar), and spherical coordinates and lesser-known ones such as elliptical cylindrical coordinates, parabolic cylindrical coordinates, prolate spheroidal coordinates, oblate spheroidal coordinates, and parabolic coordinates [Moon & Spencer, 1988]. Note that the preceeding list does not exhaust all possible coordinate systems. (There are others in $\mathbb{R}^2$ and $\mathbb{R}^3$ and the preeceding examples may be generalized to manifolds in higher dimensions for which separability is retained.) Appendix A includes a general procedure for determining if the Helmholz equation is separable for a given coordinate system.

Applying the above theorem to the radially vibrating spherical quantum billiard [Liboff & Porter, 2000], one finds that rotational symmetry between some pairs of eigenstates in the superposition is required in order for the system to exhibit chaotic behavior. That is, the azimuthal and orbital quantum numbers of two of the states in the superposition must be equal. The value of the principal quantum number n does not affect the existence of chaos.

The solution of the Schrödinger equation is of the form [Sakurai, 1994]

$$\psi(r, t) = \sum_{n=1}^{\infty} A_n \alpha_n e^{-\frac{iE_n t}{\hbar}} \psi_n(r)\,. \tag{3}$$

Absorbing the resulting time-dependence (in the phase) into the coefficient $A_n(t)$ yields

$$\psi(r, t) = \sum_{n=1}^{\infty} A_n(t) \alpha_n(t) \psi_n(r, t)\,. \tag{4}$$

In order to examine the present problem, consider a two-term superposition state of the vibrating billiard in (X, g). The results for a k-term superposition state follow from considering the terms pairwise. The superposition between the nth and qth states is given by

$$\psi_{nq}(x, t) \equiv \alpha_n A_n(t) \psi_n(x, t) + \alpha_q A_q(t) \psi_q(x, t)\,. \tag{5}$$

We substitute this wavefunction into the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(x, t),\ x \in X\,, \tag{6}$$

where the kinetic energy corresponding to the Hamiltonian of the particle confined within the billiard is given by

$$K = -\frac{\hbar^2}{2m} \nabla^2. \tag{7}$$

The total Hamiltonian of the system is given by

$$H(a_1, \ldots, a_s, P_1, \ldots, P_s) = K + \sum_{j=1}^{s} \frac{P_j^2}{2M_j} + V\,, \tag{8}$$

where $a_1, \ldots, a_s$ represent the time-varying boundary components, and the walls of the quantum billiard are in a potential V and have momenta P_j with corresponding masses M_j. The particle kinetic energy K is the quantum-mechanical (fast) component of the Hamiltonian, whereas the remainder of the Hamiltonian — representing the potential and kinetic energies of the billiard boundary — is the classical (slow) component in this semi-quantum system. We use an adiabatic (Born–Oppenheimer) approximation [Blümel & Esser, 1994] by only considering the quantum-mechanical component K of this coupled classical-quantum system as the Hamiltonian in the Schrödinger equation. The Born–Oppenheimer approximation is commonly used in mesoscopic physics. In this analysis, we also neglect Berry phase [Zwanziger *et al.*, 1990].

For the present configuration, we assume that V does not depend explicitly on time. That is,

$$V = V(a_1, \ldots, a_s)\,. \tag{9}$$

Note that we are applying nonlinear boundary conditions:

$$\psi(a_1(t), \ldots, a_s(t)) = 0\,. \tag{10}$$

Taking the expectation of both sides of (6) for the state (5) gives the following relations:

$$\left\langle \psi_{nq} \left| -\frac{\hbar^2}{2m}\nabla^2\psi_{nq} \right\rangle = K(|A_n|^2,\, |A_q|^2,\, a_1, \ldots,\, a_s)\right.$$

$$i\hbar \left\langle \psi_{nq} \left| \frac{\partial \psi_{nq}}{\partial t} \right\rangle = i\hbar[\dot{A}_n A_q^* + \dot{A}_q A_n^* + \nu_{nn}|A_n|^2\right.$$
$$+ \nu_{qq}|A_q|^2 + \nu_{nq}A_n A_q^*$$
$$+ \nu_{qn}A_q A_n^*]\,. \qquad (11)$$

In a one *dov* billiard, $a(t) \equiv a_1(t)$ is the only time-dependent boundary term (with corresponding momentum $P(t) \equiv P_1(t)$), so in this case, the kinetic energy is written

$$K = K(|A_1|^2,\, |A_2|^2,\, a)\,, \qquad (12)$$

where we use the notation $A_1 \equiv A_n$, $A_2 \equiv A_q$. The potential energy is given by

$$V = V(a)\,. \qquad (13)$$

In this case, there is a single momentum term in H given by $P^2/2M$. Liboff and Porter [2000] showed for the radially vibrating spherical billiard that if ψ_n and ψ_q do not have common angular-momentum quantum numbers, then $\mu_{nq} = \mu_{qn} = 0$, where the coupling coefficient $\mu_{nn'}$ is defined by

$$\nu_{nn'} \equiv \mu_{nn'}\frac{\dot{a}}{a}\,. \qquad (14)$$

We show that the vanishing of these coefficients in any one *dov* quantum billiard implies nonchaotic behavior of a given superposition state of that billiard. Without such cross terms, one observes that $\dot{A}_j$ is a function of only A_j and a:

$$\dot{A}_j = \chi_j(A_j,\, a)\,. \qquad (15)$$

Therefore, $|A_j(t)|^2$ is a function only of $a(t)$, and so the present system has the Hamiltonian

$$H(a,\, P) = K(a) + \frac{P^2}{2M} + V(a)\,, \qquad (16)$$

where

$$P = -i\hbar\nabla_a \equiv \hat{a}\cdot\nabla \equiv -i\hbar\frac{\partial}{\partial a} \qquad (17)$$

is the momentum of the billiard's boundary. The symbol ∇_a represents the component of the gradient in the direction $\hat{a}$. In spherical coordinates, for example, we identify $\hat{a}$ with the unit vector in the radial direction, and thus ∇_a represents the component of the gradient in the radial direction.

The Hamiltonian (16) describes an autonomous single degree-of-freedom system, which corresponds to a two-dimensional autonomous dynamical system, whose nonchaotic properties are well established [Guckenheimer & Holmer, 1983; Wiggins, 1990]. We therefore conclude that at least one of the coupling coefficients μ_{nq} or μ_{qn} must be nonzero for a quantum billiard with one *dov* to exhibit chaotic behavior. We show below for separable systems (see Appendix A) that the condition for the coupling coefficients μ_{nq} to vanish is a consequence of the orthogonality of the superposition's component functions $f_j(x_j)$ (see Eq. (A.13) in Appendix A).

In the case of a k-term superposition, one considers the coupling coefficients $\{\mu_{nq}\}$ of each pair of eigenstates in the superposition. If any one of these coupling terms is nonzero, then one expects the system to exhibit chaotic behavior. Indeed, the fact that the coupling coefficients do not vanish implies that one obtains a five-dimensional dynamical system (which is really a two degree-of-freedom Hamiltonian system in disguise). One observes numerically that no matter which two terms one considers, the resulting dynamical system behaves chaotically for some sets of parameters and initial conditions. Note that the above theorem does not hold for two *dov* quantum billiards, because if one considers an inseparable potential such as the anharmonic potential, then one has a two degree-of-freedom Hamiltonian system even for cases in which the coupling coefficient vanishes. In the next subsection, we discuss the technical details of the proof of this theorem.

2.2. *Orthogonality of the component functions*

Using the method of separation of variables (again see Eq. (A.13) in Appendix A) on the Helmholtz equation for a system with s degrees-of-freedom, one obtains s boundary-value problems to solve. (Note that the ordinary differential equations for f_j are Sturm–Liouville problems.) The solutions to such problems may be expressed as eigenfunction expansions [Butkov, 1968]. The orthogonality properties of the resulting eigenfunctions are well-known. For each j,

$$\left\langle f_j^{n_j} \left| f_j^{n_j'} \right\rangle = \delta_{n_j n_j'}\,. \qquad (18)$$

When taking the expectation of the right side of Eq. (5), the orthogonality relations satisfied by the s component functions f_j play an essential role. In the following discussion, *fb* and *mb* denote fixed boundaries and movable boundaries, respectively. When calculating the expectation, one must integrate with respect to all s variables to see when the inner product in (18) is nonzero. In particular, this inner product is present in each of the cross terms for the $(s-1)$ *fb* variables, so those terms vanish unless $n_j = n'_j$ for each of these $(s-1)$ variables. By the separability of ψ, the s-dimensional expectation integral is expressible as the product of s one-dimensional integrals, so each term includes a prefactor that consists of the product of $(s-1)$ inner products. Using the Chain Rule, one finds that a variable whose corresponding boundary is time-dependent ("*mb* variables") will manifest differently in the calculation [Liboff & Porter, 2000]. Since the *fb* variables must have corresponding symmetric *fb* quantum numbers ($n_j = n'_j$ for all $j \in \{k_1, \ldots, k_{s-1}\}$) for a two-state superposition to have nonzero coupling coefficients $\{\mu_{nq}\}$, and since we showed above that there must be at least one such cross term for a one *dov* quantum billiard to exhibit chaotic behavior, there must exist a pair of eigenstates whose $(s-1)$ *fb* quantum numbers are equal. This completes the proof of Theorem 1.

3. Quantum Billiards with Two or More Degrees-of-Vibration

We now generalize the above results to quantum billiards with vibrations of two or more degrees-of-freedom. Suppose that ξ of the s boundary components are time-dependent and also suppose that the Hamiltonian is separable:

$$H(a_1, \ldots, a_\xi, P_1, \ldots, P_\xi) = \sum_{j=1}^{\xi} H_j(a_j, P_j)\,. \quad (19)$$

For H to be separable, one requires that both the billiard's potential $V(a_1, \ldots, a_\xi)$ and the kinetic energy $K(|A_1|^2, \ldots, |A_k|^2, a_1, \ldots, a_\xi)$ be separable in the same sense as the Hamiltonian. For some systems, such as the vibrating rectangular parallelepiped, the kinetic energy is separable. For others, this need not be the case. For example, the spherical billiard has kinetic energy $K(r, \theta, \phi) = K_1(r)K_2(\theta, \phi)$, which is not equal to $K_1 + K_2$.

If, in a given superposition, there are no cross terms in the expectation (11), the ξ degree-of-freedom autonomous Hamiltonian above gives rise to a 2ξ-dimensional autonomous system, which, because of the separability, decouples into ξ two-dimensional autonomous systems, whose nonchaotic properties are well-known. If either V or K is not separable, the system does not decouple. One therefore cannot conclude that the system does not have chaotic behavior even in the absense of cross terms. A given system is very likely to behave chaotically in this event. In the separable case, then, a k-term superposition state exhibits chaotic behavior when the corresponding $(s-\xi)$ *fb* quantum numbers must be the same for some pair of eigenstates (i.e. the ith *fb* quantum number in one state must be the same as the ith *fb* quantum number in the other state of the pair. Here, i runs over all $(s-\xi)$ *fb* quantum numbers). The proof is entirely analogous to the one above.

4. Differential Equations for One Degree-of-Vibration Quantum Billiards

In the present section, we derive a general form for the coupled differential equations describing quantum billiards (in a separable coordinate system) with one *dov* and a nonvanishing coupling coefficient μ_{nq}. The resulting system of ordinary differential equations behaves chaotically. Indeed, numerical simulations indicate chaotic behavior for some choices of initial conditions and parameters.

Theorem 2. *Consider a one dov quantum billiard with the same geometric conditions as in Theorem 1. Let the point particle inside the billiard be of mass m_0, the mass of the billiard's boundary be $M \gg m_0$, and the surface potential of the billiard be $V = V(a)$, where $a = a(t)$. For a two-term superposition, if the ith fb quantum number is the same in both states (where i runs over all $(s-1)$ of these numbers), then the system of differential equations describing the evolution of the superposition state has the following form in terms of Bloch variables x, y, z (defined below) [Allen & Eberly, 1987], displacement a, and momentum P*:

$$\dot{x} = -\frac{\omega_0 y}{a^2} - \frac{2\mu_{qq'} P z}{Ma}\,, \quad (20)$$

$$\dot{y} = \frac{\omega_0 x}{a^2}\,, \quad (21)$$

$$\dot{z} = \frac{2\mu_{qq'} P x}{Ma}\,, \quad (22)$$

$$\dot{a} = \frac{P}{M}\,, \tag{23}$$

and

$$\dot{P} = -\frac{\partial V}{\partial a} + \frac{2[\varepsilon_+ + \varepsilon_-(z - \mu_{qq'}x)]}{a^3}\,. \tag{24}$$

In the above equations,

$$\omega_0 \equiv \frac{\varepsilon_{q'} - \varepsilon_q}{\hbar}\,, \tag{25}$$

and

$$\varepsilon_\pm \equiv \frac{(\varepsilon_{q'} \pm \varepsilon_q)}{2}\,, \tag{26}$$

where ε_q and $\varepsilon_{q'}$ $(q \neq q')$ are the coefficients in the kinetic energy corresponding to the mb quantum numbers. Additionally, x, y and z represent (dimensionless) Bloch variables:

$$x = \rho_{12} + \rho_{21}\,, \tag{27}$$

$$y = i(\rho_{21} - \rho_{12})\,, \tag{27'}$$

$$z = \rho_{22} - \rho_{11}\,, \tag{27''}$$

where the density matrix is defined by $\rho_{qn} = A_q A_n^*$ [Liboff, 1998].

Before we begin the proof of Theorem 2, note that the differential equations describing the evolution of a two-term superposition state are of the above form for the linear vibrating billiard [Blümel & Esser, 1994; Blümel & Reinhardt, 1997] as well as for the vibrating spherical billiard with both vanishing and nonvanishing angular momentum eigenstates [Liboff & Porter, 2000]. Recall that this system of equations has two constants of motion. They are the energy (Hamiltonian)

$$H = \text{constant} \tag{28}$$

and the radius of the Bloch sphere

$$x^2 + y^2 + z^2 = 1\,, \tag{29}$$

so there are three independent dynamical variables in the set $\{x, y, z, a, P\}$.

We verify Theorem 2 using techniques from Riemannian geometry. It is well known that for s-dimensional Riemannian manifolds, the volume element dV has units of (distance)^s, which may include some "prefactors." (For example, in cylindrical coordinates, $dV = rdrd\theta dz$, where r is the prefactor.) In particular, if there are ξ "angular variables" (dimensionless quantities, like θ in the above example), there will be a prefactor that includes the term r^ξ so that the volume element has appropriate dimensions. Additionally, in a quantum billiard with one *dov* corresponding to the boundary dimension $a(t)$, the wave-function has a normalization factor of order $a^{-\sigma/2}$, where σ corresponds to the number of distance dimensions affected by the vibration, which is a different concept from the *dov*. For example, in the radially vibrating sphere, the vibration of the radius affects three dimensions, even though this system has one *dov*. In contrast, for a rectangle in which either the length or width (but not both) is time-dependent, a single distance dimension is affected, and the *dov* is also one. When taking the expectation of the Schrödinger equation (6), the normalization prefactor of ψ is squared, which gives a factor of $a^{-\sigma}$. We perform s inner products (and hence s integrations) in taking this expectation, which gives a factor of $\dot{a}/a$ in each of the cross terms, as was the case for known examples [do Carmo, 1992; Abraham *et al.*, 1988]. The diagonal terms in the expectation (11) are due only to the kinetic energy, because of orthogonality conditions on the wavefunctions ψ_q and $\psi_{q'}$.

The evolution equations for $\dot{A}_1$ and $\dot{A}_2$ (see Eq. (5), *etc.*) are thus

$$i\dot{A}_n = \sum_{j=1}^{2} D_{nj} A_j, \tag{30}$$

where

$$(D_{nj}) = \begin{pmatrix} \dfrac{\varepsilon_q}{\hbar a^2} & -i\mu\dfrac{\dot{a}}{a} \\ i\mu\dfrac{\dot{a}}{a} & \dfrac{\varepsilon_{q'}}{\hbar a^2} \end{pmatrix}, \tag{31}$$

and $\mu \equiv \mu_{qq'} = -\mu_{q'q} \neq 0$ is a coupling coefficient (proportional to $\nu_{qq'}$) for the cross term $A_q A_{q'}^*$ corresponding to Eq. (11). Transforming these amplitudes to Bloch variables (27) completes the proof of Theorem 2. The calculation is exactly as in the radially vibrating spherical billiard [Liboff & Porter, 2000].

The above equations may be used to illustrate KAM theory [Guckenheimer & Holmes, 1983; Wiggins, 1990; Katok & Hasselblatt, 1995]. Toward that purpose, the number of nonresonant tori that have broken up depends on the initial condition of a given integral curve. One may obtain, for example, periodic and quasiperiodic orbits (corresponding to closed curves in the Poincaré map) as

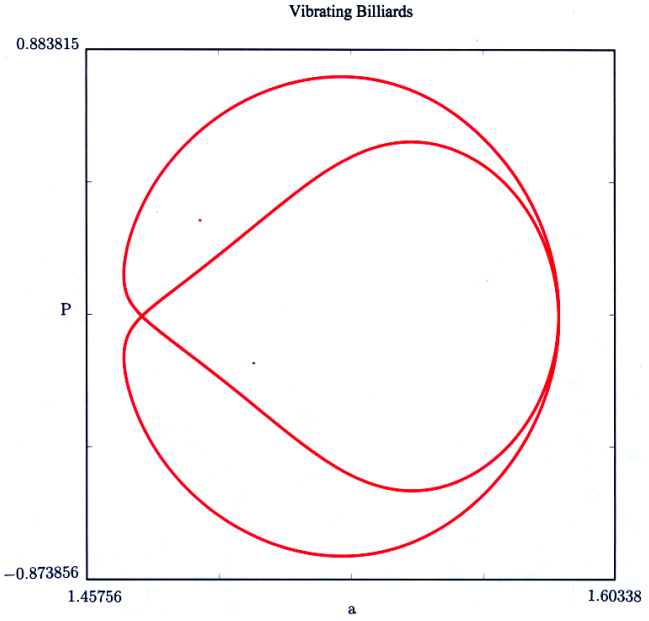

Fig. 1. Periodicity and quasiperiodicity I in a one *dov* quantum billiard.

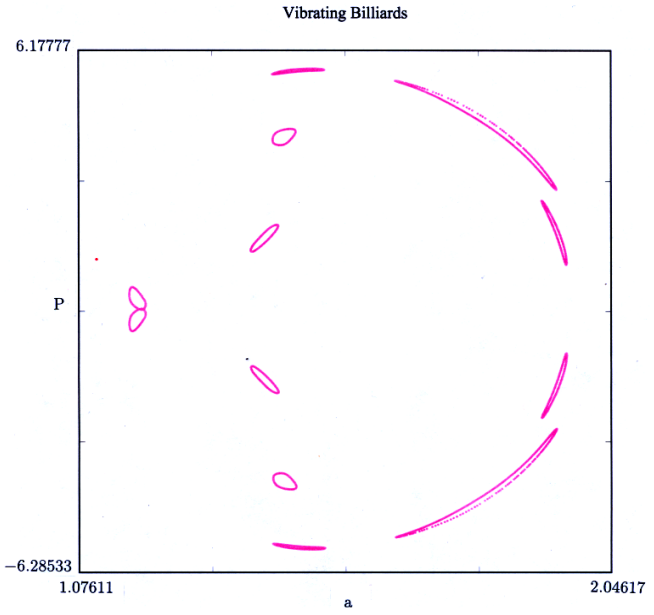

Fig. 2. Periodicity and quasiperiodicity II in a one *dov* quantum billiard.

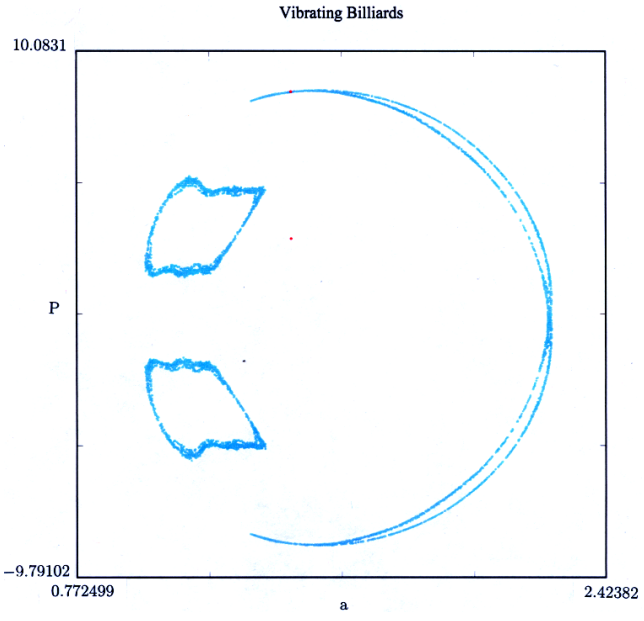

Fig. 3. Local chaos in a one *dov* quantum billiard.

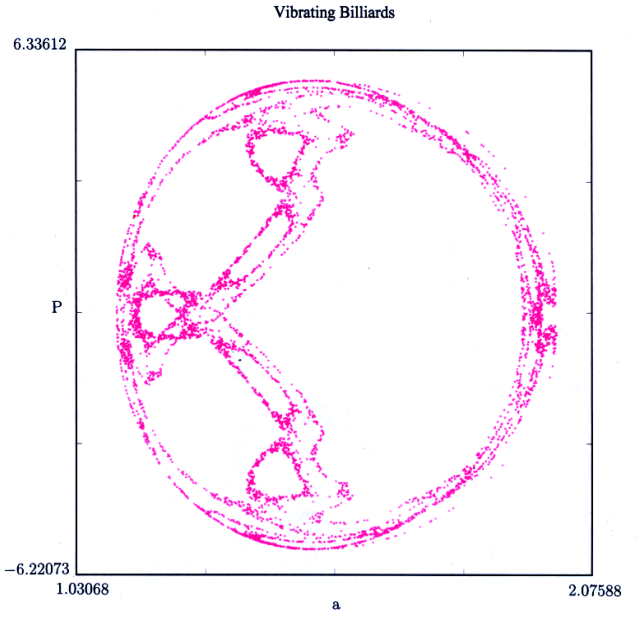

Fig. 4. Structured global chaos in a one *dov* quantum billiard.

in Figs. 1 and 2, local ("soft") chaos (in which these closed curves become "fuzzy") as in Fig. 3, structured global chaos (Fig. 4), islands of order in a sea of chaos (Fig. 5), and finally global chaos (Fig. 6). The Poincaré sections corresponding to the descriptions above for the evolution equations of a one *dov* quantum billiard have initial conditions and parameter values $x(0) = \sin(0.95\pi) \approx 0.15643446504$, $y(0) = 0$, $z(0) = \cos(0.95\pi) \approx -0.987688340595$, $V_0/a_0^2 = 5$, $a_0 = 1.25$, $\hbar = 1$, $\varepsilon_1 = 5$, $\varepsilon_2 = 10$, and $\mu = 1.5$. Figures 1–6 are plots for the harmonic potential

$$V = \frac{V_0}{a_0^2}(a - a_0)^2 \,. \tag{32}$$

5. Phenomenology

We now discuss the phenomenology of quantum chaos in the present context. In the language

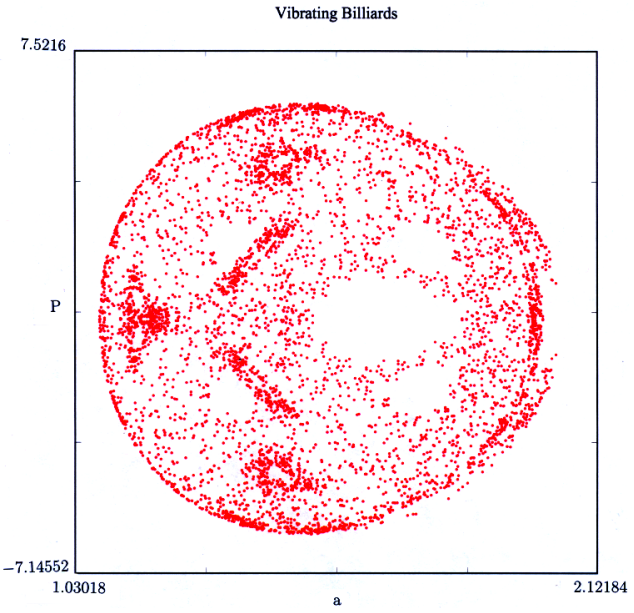

Fig. 5. Islands in a sea of chaos in a one *dov* quantum billiard.

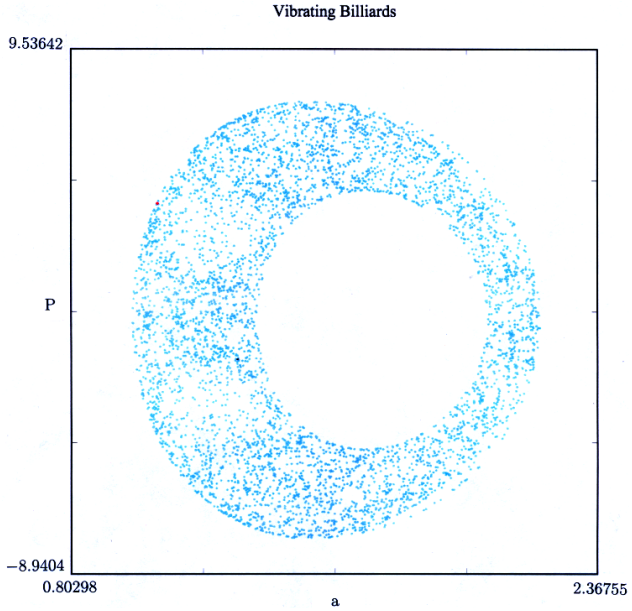

Fig. 6. Global chaos in a one *dov* quantum billiard.

of Blümel and Reinhardt [1997], vibrating quantum billiards are an example of semiquantum chaos, which describes different behavior than the so-called "quantized chaos" that is more commonly studied. Quantized chaos or "quantum chaology" is the study of the quantum signatures of classically chaotic systems, usually in the semiclassical ($\hbar \to 0$) or high quantum-number limits. The observed behavior in these studies is not strictly chaotic, but the nonintegrability of these systems is nevertheless evident. The fact that their classical analogs are genuinely chaotic has a notable effect on the quantum dynamics [Liboff, 2000]. In the semiquantum chaotic situation, the semiclassical and high quantum-number limits are unnecessary and the observed behavior is genuinely chaotic.

In vibrating quantum billiards, one has a classical system (the walls of the billiard) coupled to a quantum-mechanical one (the particle enclosed by the billiard boundary). Considered individually, each of these subsystems is integrable. When they are coupled, however, one observes chaotic behavior in each of them. (Physically, the coupling occurs when the particle confined within the billiard strikes the vibrating boundary. The motions of the particle and wall thereby affect each other.) The classical variables (a, P) exhibit Hamiltonian chaos, whereas the quantum subsystem (x, y, z) is truly quantum chaotic. Chaos on the Bloch sphere is an example of quantum chaos, because the Bloch variables (x, y, z) correspond to the quantum probabilities of the wavefunction. Additionally, a single normal mode depends on the radius $a(t)$, and so each eigenfunction is an example of quantum-mechanical wave chaos for the chaotic configurations of the billiard. Because the evolution of the probabilities $|A_i|^2$ is chaotic, the wavefunction ψ in the present configuration is a chaotic combination of chaotic normal modes. This is clearly a manifestation of quantum chaos. Finally, we note that if we quantized the motion of the billiard's walls, we would obtain a higher-dimensional, fully-quantized system that exhibits quantized chaos [Blümel & Reinhardt, 1997]. In particular, the fully quantized version of the present system would require passage to the semiclassical limit in order to observe quantum signatures of classical chaos.

6. Conclusions

We derived necessary conditions for the existence of chaos in one degree-of-vibration quantum billiards on Riemannian manifolds (Theorem 1). In a k-state superposition, there must exist a pair of states whose fb quantum numbers are pairwise equal. The results of this theorem arise from the separability of the Schrödinger equation for a given orthogonal coordinate system as well as orthogonality relations satisfied by solutions of the Schrödinger equation. We also discussed a generalization of the previous result to vibrating quantum billiards with two or

more *dov*. Moreover, we derived a general form (Theorem 2) for the coupled equations that describe vibrating quantum billiards with one *dov*, and we used these equations to illustrate KAM theory.

We showed that the equations of motion (20)–(24) for a one *dov* quantum billiard describe a class of problems that exhibit semiquantum chaotic behavior [Blümel & Esser, 1994; Blümel & Reinhardt, 1997; Liboff & Porter, 2000]. Unlike in quantum chaology, the behavior in question is genuinely chaotic. Additionally, we did not need to pass to the semi-classical ($\hbar \to 0$) or high quantum-number limits in order to observe such behavior. From a more practical standpoint, the radially vibrating spherical billiard may be used as a model for particle behavior in the nucleus [Wong, 1990], the "quantum dot" nanostructure [Lucan, 1998], and the Fermi accelerating sphere [Badrinarayanan & Jose, 1995]. The vibrating cylindrical billiard may be used as a model of the "quantum wire" microdevice component [Liboff, 1998; Zaren *et al.*, 1989]. At low temperatures, quantum-well nanostructures experience vibrations due to zero-point motions, and at high temperatures, they vibrate because of natural fluctuations. Additionally, the "liquid drop" and "collective" models of the nucleus include boundary vibrations [Wong, 1990]. The present paper thus has both theoretical and practical import because it expands the mathematical theory of quantum chaos and has application in nuclear, atomic, and mesoscopic physics.

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Appendix A
Separability of the Helmholtz Operator

Consider an s-dimensional Riemannian manifold with metric coefficients $\{g_{11}, \ldots, g_{ss}\}$ defined by

$$g_{jj} = \sum_{i=1}^{s} \left(\frac{\partial x_i}{\partial u_j} \right)^2 , \tag{A.1}$$

where x_i represents the ith rectangular coordinate and u_j represents the distance along the jth axis [Zwillinger, 1996]. The Riemannian metric is then $g = \prod_{j=1}^{s} g_{jj}$. For notational convenience, one defines $h_j = \sqrt{g_{jj}}$, so that $\sqrt{g} = \prod_{j=1}^{s} h_j$. In cylindrical coordinates in $\mathbb{R}^3$, for example, $x_1 = r\cos(\theta)$, $x_2 = r\sin(\theta)$ and $x_3 = z$, so that one obtains $h_1 = 1$, $h_2 = r$ and $h_3 = 1$.

We review the following analysis from Riemannian geometry so that the proof of Theorem 1 is easier to follow. To express the Helmholtz equation on (X, g), one writes the Laplace–Beltrami operator ∇^2 with respect to the metric g:

$$\nabla^2 = \frac{1}{\sqrt{g}} \sum_{j=1}^{s} \frac{\partial}{\partial u_j} \left(\frac{\sqrt{g}}{g_{jj}} \frac{\partial}{\partial u_j} \right) . \tag{A.2}$$

If the manifold X is three-dimensional, the Laplacian takes the form

$$\begin{aligned} \nabla^2 &= \frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial u_1} \left(\frac{\sqrt{g}}{g_{11}} \frac{\partial}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{\sqrt{g}}{g_{22}} \frac{\partial}{\partial u_2} \right) \right. \\ &\quad \left. + \frac{\partial}{\partial u_3} \left(\frac{\sqrt{g}}{g_{33}} \frac{\partial}{\partial u_3} \right) \right] \\ &= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial}{\partial u_2} \right) \right. \\ &\quad \left. + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial}{\partial u_3} \right) \right] . \end{aligned} \tag{A.3}$$

We now discuss the separability of the Helmholtz equation $\nabla^2\psi + \lambda^2\psi = 0$, which is one of our geometrical conditions. To do so, define the Stäckel matrix [Benenti, 1980; Moon & Spencer, 1988]

$$S \equiv (\Phi_{ij}) , \tag{A.4}$$

where $\Phi_{ij} = \Phi_{ij}(u_i)$, and the $\{\Phi_{ij}\}$ are specified by the following procedure. Define

$$C \equiv \det(S) = \sum_{j=1}^{s} \Phi_{j1} M_{j1} . \tag{A.5}$$

In the preceeding equation, the $(j, 1)$-cofactor M_{j1} is given by

$$M_{j1} = (-1)^{j+1} \det[M(j|1)] , \tag{A.6}$$

where $M(j|i)$ represents the (j, i)-cofactor matrix that one obtains by considering the submatrix of S defined by deleting the jth row and the ith column [Strange, 1988]. In three dimensions, M_{j1} take the form

$$M_{11} = \begin{vmatrix} \Phi_{22} & \Phi_{23} \\ \Phi_{32} & \Phi_{33} \end{vmatrix} , \tag{A.7}$$

$$-M_{21} = \begin{vmatrix} \Phi_{12} & \Phi_{13} \\ \Phi_{32} & \Phi_{33} \end{vmatrix} , \tag{A.8}$$

and

$$M_{31} = \begin{vmatrix} \Phi_{12} & \Phi_{13} \\ \Phi_{22} & \Phi_{23} \end{vmatrix} . \tag{A.9}$$

If

$$g_{jj} = \frac{C}{M_{j1}} \tag{A.10}$$

and

$$\frac{\sqrt{g}}{C} = \prod_{j=1}^{s} \eta_j(u_j) , \tag{A.11}$$

then the solution of the Helmholtz equation

$$\nabla^2\psi + \lambda^2\psi = 0 \tag{A.12}$$

separates

$$\psi = \prod_{j=1}^{s} f_j(u_j)\,, \tag{A.13}$$

where f_j solves the Sturm–Liouville equation [Simmons, 1991]

$$\frac{1}{\eta_j}\frac{d}{du_j}\left(\eta_j \frac{df_j}{du_j}\right) + f_j \sum_{i=1}^{s} b_i \Phi_{ji} = 0,\ j \in \{1, \ldots, s\}\,. \tag{A.14}$$

In (A.14), $b_1 = \lambda^2$, and all other b_i are arbitrary. For a given Stäckel matrix, this prescribes the $\{\eta_j\}$ for which the separability conditions hold. It is important to note that for a given metric g, the choice of the Stäckel matrix is not unique and that for some metrics, there is no Stäckel matrix that can be chosen and hence no way to separate the Helmholtz operator. Note also that the time-dependent Schrödinger equation is separable whenever the Helmholtz equation is separable.

As a special case [corresponding to $\lambda = 0$ in (A.12)], Laplace's equation is separable whenever

$$\frac{g_{jj}}{g_{kk}} = \frac{M_{k1}}{M_{j1}} \tag{A.15}$$

and

$$\frac{\sqrt{g}}{g_{jj}} = M_{j1} \prod_{i=1}^{s} \eta_i(u_i), \quad j,\, k \in \{1, \ldots, s\}. \tag{A.16}$$

Note that the preceeding condition does not completely decribe the separability of the Helmholtz operator, because although the Helmholtz equation is separable whenever the Laplacian is separable, the converse is not true.

Appendix B
Galërkin Approximations

The method used to obtain nonlinear coupled ordinary differential equations for the amplitudes A_j amounts to applying the Galërkin method [Guckenheimer & Holmes, 1983; Temam, 1997] to the Schrödinger equation, an infinite-dimensional dynamical system. It has been used for many years to study nonlinear reaction–diffusion equations that occur in fluid mechanics. It can also be used in the study of nonlinear Schrödinger equations (NLS). Our treatment of the linear Schrödinger equation with nonlinear boundary conditions thus parallels established methods for nonlinear partial differential equations. Additionally, the Finite Element Method is also based on a Galërkin approximation [Johnson, 1987] and one can use such methods in inertial manifold theory.

The Galërkin method proceeds as follows. Consider a partial differential equation (possibly nonlinear) whose solution is the function ψ. Express ψ as an expansion in some orthonormal set of eigenfunctions $\psi_i(x)$, $i \in I$:

$$\psi(x) = \sum_{I} c_i(\overline{x})\psi_i(x), \quad x \in X\,, \tag{B.1}$$

where I is any indexing set and the coefficients $c_i(\overline{x})$ are unknown functions of some but not all of the independent variables in the vector x, as in the present paper. This gives a countably infinite coupled system of nonlinear ordinary differential equations for $c_i(\overline{x})$, $i \in I$. (If the partial differential equation is linear with linear boundary conditions, then taking an eigenfunction expansion gives constant coefficients $c_i(\overline{x}) \equiv c_i$.) One then projects the expansion (49) onto a finite-dimensional space (by assuming that only a certain finite subset of the $c_i(\overline{x})$ are nonzero) to obtain a finite system of coupled ordinary differential equations. Thus, a two-term superposition state corresponds to a two-term Galërkin projection. If all the dynamical behavior of a system lies on such a finite-dimensional projection, then one has found an inertial manifold of the system [Temam, 1997].