

Is semiquantum chaos real?

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A semiquantum system, composed of a quantum part coupled to a classical part, can exhibit dynamical chaos in the motion of the quantum state vector. However, there has been disagreement as to whether this mathematical chaos is physically real or merely an artifact of the semiquantum approximation. It is shown, for a model of a quantum spin coupled to an approximately classical nonlinear oscillator, that the semiquantum chaos disappears rapidly as the mass of the oscillator is increased to make it more classical. The time interval during which the semiquantum approximation remains accurate increases with the mass, but is not closely related to the Lyapunov time.

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I. INTRODUCTION

Classical chaos may be defined as extreme complexity of the trajectories in phase space, with the trajectories being very sensitive to small changes in the initial conditions. Its characteristic manifestations include a seemingly random distribution of phase points on the Poincaré surface of section, and an exponentially rapid separation of two initially close trajectories (measured by a positive Lyapunov exponent) [1]. It is well known that the state vector of a closed quantum system does not exhibit chaotic motion in Hilbert space. This is evident from the fact that the inner product $\langle \psi_1(t) | \psi_2(t) \rangle$, and hence also the metric distance, between two state vectors in Hilbert space is constant, as a consequence of the unitary nature of time evolution. However, the coupling of a quantum system to a classical system can lead to a genuinely chaotic motion of the quantum state in its Hilbert space, a phenomenon known as *semiquantum chaos* [2,3]. This term is reserved for systems in which neither the quantum part nor the classical part would be chaotic by itself, and the chaos is a result of the coupling between them.

Semiquantum models arise in the Born-Oppenheimer approximation if the system divides naturally into a fast (quantum) part and a slow (approximately classical) part. Blümel *et al.* [2,4] studied in detail a model consisting of a quantum part whose boundaries are directly coupled to a classical part, with the expectation value of the quantum energy acting as an effective potential for the classical part. The mutual coupling of the quantum and classical parts leads to chaotic motions. Similar phenomena are predicted for a (quantum) atom interacting with a (classical) cavity field [5–8]. The essential structure of all these models (including the model used in this paper) is a classical part acting directly on the quantum part, with the quantum part reacting back on the classical part through the expectation value of some observable. With appropriate nonlinearity in either the coupling or the internal dynamics of the classical part, such a model can exhibit chaos.

Although these systems, as *mathematical* models, do indeed exhibit chaos, there is some doubt as to whether that prediction corresponds to physical reality. Treating part of the system as classical is surely an approximation. What would happen to the semiquantum prediction of chaos if both

parts of the system were treated by quantum mechanics without approximation? On the one hand, we have the theorem [9] that the state of a closed quantum system is at most quasiperiodic in Hilbert space, which argues against the reality of semiquantum chaos. But what about the quantum state of only one part of the system when the other part is approximately classical? Perhaps semiquantum chaos is real in the regime where that approximation is accurate. Blümel *et al.* [10] argue for the reality of semiquantum chaos. Others [11], however, have argued that the classical approximation is valid only for times too short to see the chaos, and that the predicted chaos is an artifact of the approximation.

A limitation of most previous calculations of semiquantum chaos has been the failure to identify and systematically vary any parameter that controls the degree of classicality. That omission is remedied in this paper, where the mass of one part is varied to make it more classical. We find that as the classical part of the system becomes more massive, more macroscopic, and hence more accurately classical, the microscopic quantum part has a diminishing effect on it, and eventually becomes too weak to drive the system to chaos. The extent to which the results for this model may be typical of semiquantum systems is discussed in the final section of this paper.

It should be emphasized that the problem studied in this paper, namely whether or not chaotic motion in the Hilbert space of a semiquantum system exists, is distinct from the more fundamental problem of the emergence of classical chaos in a closed quantum system whose classical counterpart is chaotic. Chaos emerges from quantum mechanics in the classical limit, not from any chaotic motion of the state vector through Hilbert space, but rather from the growth of complex structures in the probability distributions that are described by the state vector [12].

II. THE SPIN-PARTICLE MODEL

The model studied in this paper consists of a quantum spin $\vec{\sigma}$ interacting with the motion of a particle. Its Hamiltonian is

$$H = B\sigma_z + Cx\sigma_x + p^2/2m + V(x). \quad (1)$$

The first term on the right is the spin Hamiltonian, the last two terms comprise the particle Hamiltonian, and second term is the interaction between the spin and the position of the particle. A quartic potential, $V(x)=x^4/4$, has been chosen for this work because it is known that a periodic driving force can drive the particle into chaotic motion in such a potential. The dynamical problem can now be solved at two different levels of treatment.

A. Full quantum theory

The time-dependent Schrödinger equation,

$$\partial/\partial t|\Psi(x,t)\rangle = -(i/\hbar)H|\Psi(x,t)\rangle, \quad (2)$$

can be solved numerically, with the momentum operator p in Eq. (1) being $-i\hbar\partial/\partial x$. Here $|\Psi(x,t)\rangle$ is a two-component state vector, and the spin operators in Eq. (1) are 2×2 Pauli matrices. The partial differential equation was solved by discretizing the coordinate x into 513 values, and solving the resultant set of 1026 coupled ordinary differential equations by standard numerical methods. The partial state of the spin can then be computed by integrating over the position variable,

$$\rho = \int |\Psi(x,t)\rangle\langle\Psi(x,t)|dx. \quad (3)$$

For spin $s=\frac{1}{2}$, the 2×2 density matrix ρ is completely described by the three components of spin polarization,

$$a_x \equiv \langle\sigma_x\rangle = \text{tr}(\rho\sigma_x), \quad (4a)$$

$$a_y \equiv \langle\sigma_y\rangle = \text{tr}(\rho\sigma_y), \quad (4b)$$

$$a_z \equiv \langle\sigma_z\rangle = \text{tr}(\rho\sigma_z), \quad (4c)$$

B. Semiquantum theory

This approximation is most easily derived from the Heisenberg equation of motion,

$$dR/dt = (i/\hbar)[H,R], \quad (5)$$

where R is the operator for one of the dynamical variables of the model, $\{\sigma_x, \sigma_y, \sigma_z, x, p\}$. The semiquantum equations are then obtained by replacing the quantum operators x and p with classical variables X and P . Since the spin operators appear only linearly in these equations, we may average them in the spin state and obtain equations of motion for the components of the spin polarization (4) coupled to the classical position and momentum variables:

$$da_x/dt = -2Ba_y, \quad (6)$$

$$da_y/dt = 2Ba_x - 2CXa_z, \quad (7)$$

$$da_z/dt = 2CXa_y, \quad (8)$$

$$dX/dt = P/m, \quad (9)$$

$$dP/dt = -X^3 - Ca_x. \quad (10)$$

It is easily verified that Eqs. (6)–(10) have two constants of motion: the total energy and the magnitude of the polarization vector $|\vec{a}|$. The polarization vector $\vec{a}=(a_x, a_y, a_z)$ provides a complete parametrization of the quantum spin-state operator, $\rho = \frac{1}{2}(I + \vec{a} \cdot \vec{\sigma})$.

C. Significant parameters of the model

Since the spin is to remain a quantum system while the particle approaches its classical limit, we set $\hbar=1$ and increase the particle mass m to make the particle more nearly classical. Thus the energy and time scales are fixed by the parameter B in the spin Hamiltonian.

Two dimensionless ratios that describe the degree of classicality of the particle can be identified. The first is the ratio of the energy-level spacings of the particle and of the spin in the absence of interaction,

$$\eta = \frac{\Delta E_p}{\Delta E_s}. \quad (11)$$

If the particle were truly classical, its energy would be continuous, and so η should be small in the semiquantum limit. Ignoring all numerical factors such as 2 and π leads to the following order of magnitude (see the Appendix):

$$\eta \approx \frac{E_p^{1/4}\hbar}{B\sqrt{m}}, \quad (12)$$

where E_p is the energy of the particle.

The second is the ratio of the deBroglie wavelength of the particle to the diameter of its orbit,

$$\Lambda = \lambda_{\text{DB}}/X_0. \quad (13)$$

A similar order-of-magnitude estimate (see the Appendix) yields

$$\Lambda \approx \frac{E_p^{-3/4}\hbar}{\sqrt{m}}. \quad (14)$$

This same magnitude is also of the ratio of \hbar to the action of the orbit. The parameters η and Λ are dimensionless, in spite of appearances, because the choice of the potential, $V(x)=x^4/4$, requires energy to be in units of (length)⁴.

These two dimensionless ratios measure the classicality of the particle in quite different ways: η measures how classical the particle is relative to the spin, while Λ measures the classicality of the particle without regard to the spin. The interaction strength C is not related to the degree of classicality, and may be fixed independently.

III. DISAPPEARANCE OF CHAOS AS $m \rightarrow \infty$

Although the polarization vector \vec{a} is to be interpreted as describing the quantum state of the spin, nevertheless the semiquantum equations (6)–(10) have the mathematical form of a classical dynamical system, to which the usual techniques may be applied. Since the length $|\vec{a}|$ of the polarization vector remains constant, it is natural to consider the

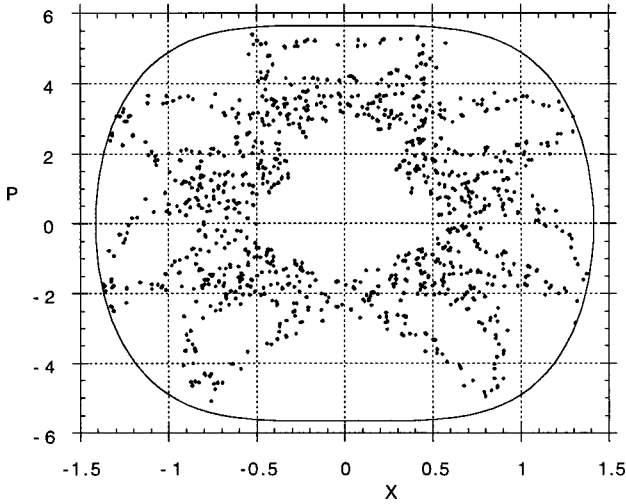


FIG. 1. Poincaré section $a_x=0$ for $E=B=0.5$, $C=1.0$, $m=16$, showing chaos in the X - P phase plane. The white spaces contain many invariant tori, which are not plotted to avoid overcomplicating the diagram.

system to have a four-dimensional phase space, $S^2 \times E^2$, formed by the surface of the spin sphere and the phase plane of the particle. Energy conservation reduces the dimension of the accessible manifold to 3, and so one further constraint yields a Poincaré surface of section.

The semiclassical limit involves $m \rightarrow \infty$, and so we expect that η [Eq. (12)] and Λ [Eq. (14)] should go to zero. But the relative magnitudes of η and Λ must be specified to define a definite limit process. It seems natural to hold constant the ratio $\eta/\Lambda = E_p/B$. Apart from a numerical factor, this is the ratio of the particle energy E_p to the spin energy E_s . The chance for complex behavior is greatest if E_s and E_p are similar in magnitude and each part has as much accessible phase space as possible. Now if the total energy $E = E_s + E_p$ is less than B , then the full sphere S^2 will not be energetically accessible to the spin. If, on the other hand, the energy E is greater than B , then a region of the X - P phase plane around the origin will be energetically inaccessible to the particle. Therefore, we choose $E=B$ as the most favorable case to study.

Figure 1 shows the Poincaré section for $a_x=0$ with a_x moving in the positive direction for a particle of mass $m=16$. The phase points fill most of the energetically accessible region (bounded by the solid curve) in a pattern typical of chaos, although there are several holes in the chaotic region that contain tori of regular trajectories. In Fig. 2, the Poincaré section $X=0$ (moving positively) is shown on the spin sphere, from which we see that the polarization vector (equivalently the quantum spin state) has a chaotic pattern covering much of the sphere. This is a clear case of semiclassical chaos.

As the mass of the particle increases, the relative size of the chaotic zone decreases. In Fig. 3, for $m=64$ it has shrunk to a thin separatrix layer. Figure 4 confirms that the spin state is also confined to a thin separatrix layer. Thus we see that chaos disappears rapidly as the mass m increases.

The width of the chaotic separatrix layer was investigated

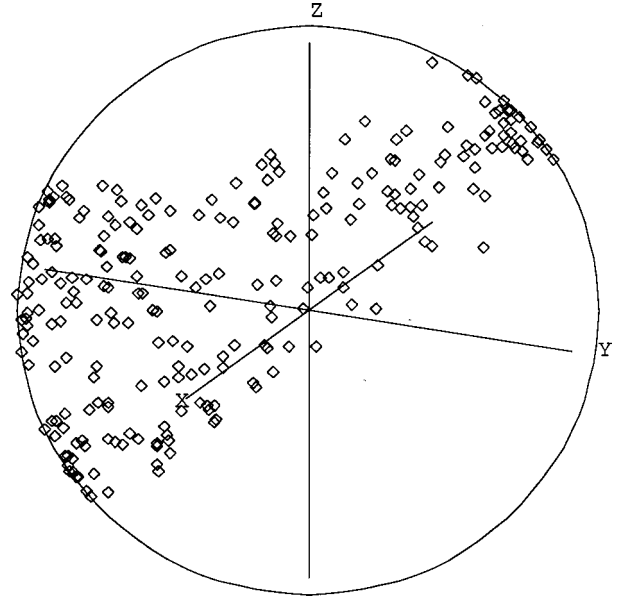


FIG. 2. Poincaré section $X=0$ for $E=B=0.5$, $C=1.0$, $m=16$, showing chaos on the spin sphere.

by Zaslavsky *et al.* [13] for a nonlinear oscillator of frequency ω driven by a perturbation of frequency ν . For $\nu \gg \omega$, they found the width of the chaotic layer to be proportional to $\exp(-\pi\nu/2\omega)$. In our model, ω would be the natural frequency of the particle and ν would be the precession frequency of the spin ($\nu=2B/\hbar$), both calculated without interaction ($C=0$). As m increases, the oscillator frequency ω decreases, and the exponential factor becomes very small. Thus the rapid disappearance of the chaotic zone is expected to be typical of the semiclassical limit, even if the limit were

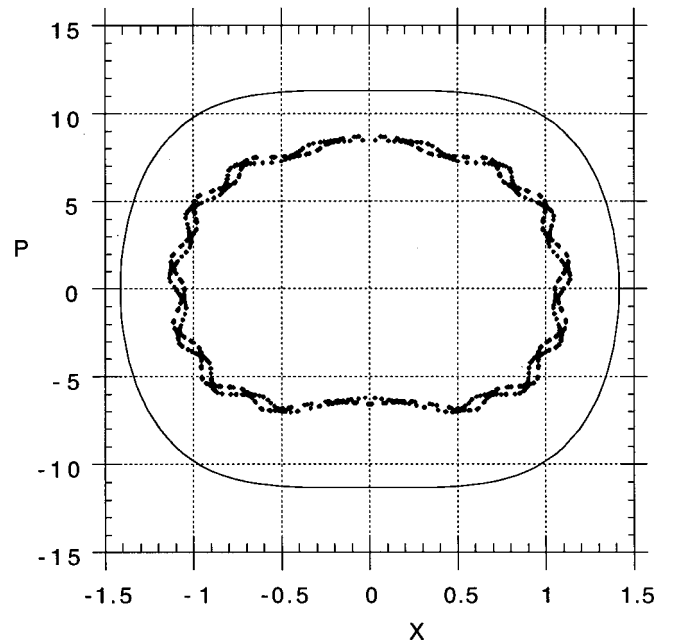


FIG. 3. Poincaré section $a_x=0$ for $E=B=0.5$, $C=1.0$, $m=64$, showing a narrow separatrix layer in the X - P phase plane. The solid curve bounds the energetically accessible region.

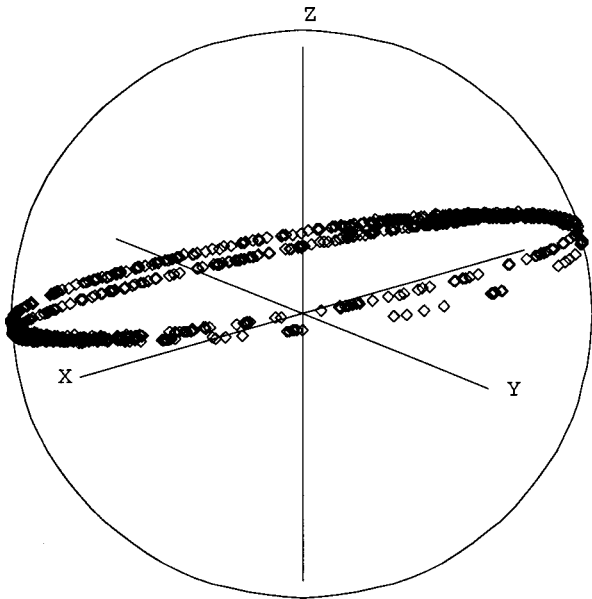


FIG. 4. Poincaré section $X=0$ for $E=B=0.5$, $C=1.0$, $m=64$, showing a narrow separatrix layer on the spin sphere.

approached by a different route from the one that we have chosen ($\eta/\Lambda = \text{const}$).

An exception to this argument occurs if we keep ν/ω constant and in resonance as $m \rightarrow \infty$. There are close connections between resonance and chaos [14], so this possibility should be studied. From the definition (11), it follows that $\eta = \hbar\omega/\hbar\nu$. Therefore, to stay in resonance, we must take the limit $\Lambda \rightarrow 0$ with η constant. This illustrates a limitation of the semiquantum theory. From a quantum point of view, we would like the energy-level spacing ΔE_p to go to zero (hence $\eta \rightarrow 0$), but from a classical point of view we want the frequency ratio to remain constant (hence $\eta = \text{const}$). We cannot do both at the same time; we have tried the first, and will now try the second, choosing the frequency ratio $\nu/\omega = 3/1$.

For a quartic potential, the oscillation frequency ω is proportional to the amplitude of oscillation X_0 [15], and since ω is also proportional to $m^{-1/2}$, we must scale the amplitude so that X_0^2/m is constant. The particle energy, which is proportional to X_0^4 , now increases very rapidly with m , and is confined within the band $E_p = E \pm B$. Figure 5 shows the $a_x = 0$ Poincaré section for $m=16$. The chaotic zone fills most of the energetically accessible band. Figure 6 shows that the spin state is also chaotic, covering most of the sphere. For $m=64$, the particle energy is much larger, and the relative width of the energetically allowed band is so small that the analog of Fig. 5 would be uninformative. However Fig. 7 shows that the motion of the spin state is quasiperiodic, being confined to a curve on the spin sphere.

Finally, we have computed the largest Lyapunov exponent λ of the system (6)–(10), using a program based upon that of Wolf *et al.* [16]. It is apparent from Fig. 8 that, as $m \rightarrow \infty$, λ rapidly becomes so small that it is difficult to distinguish it from zero. This clearly demonstrates the disappearance of semiquantum chaos in the limit in which the semiquantum approximation becomes valid.

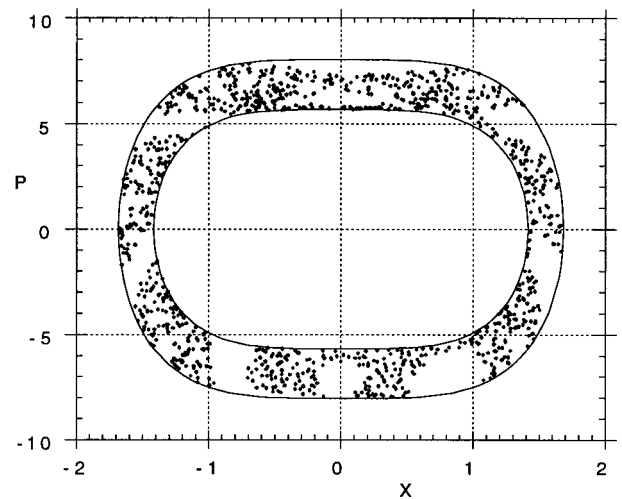


FIG. 5. Poincaré section $a_x=0$ for the 3:1 resonance, with $E=1.50659$, $B=0.5$, $C=1.0$, $m=16$. The solid curves bound the energetically accessible region.

IV. COMPARISON BETWEEN SEMIQUANTUM AND FULL QUANTUM THEORIES

In the full quantum theory, the state vector of the spin-particle system becomes entangled because of the interaction. Therefore, the partial state ρ of the spin (3) does not remain a pure state, and the spin-polarization vector \vec{a} is not confined to the surface of the unit sphere. Figure 9 illustrates the complicated (but not chaotic) motion of the polarization vector in three dimensions. The initial state is the product of a spin state with polarization $\vec{a} = (0, -1, 0)$ and a Gaussian wave packet centered at average position $\langle x \rangle = 1.18921$, with half-width $\sigma \equiv \langle (x - \langle x \rangle)^2 \rangle^{1/2} = 1.0$ and average momentum $\langle p \rangle = 0$.

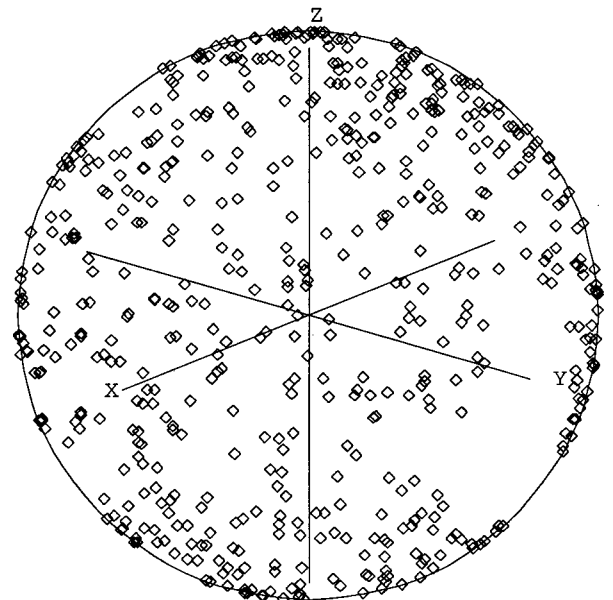


FIG. 6. Poincaré section $X=0$ for the 3:1 resonance, with $E=1.50659$, $B=0.5$, $C=1.0$, $m=16$, showing chaos on the spin sphere.

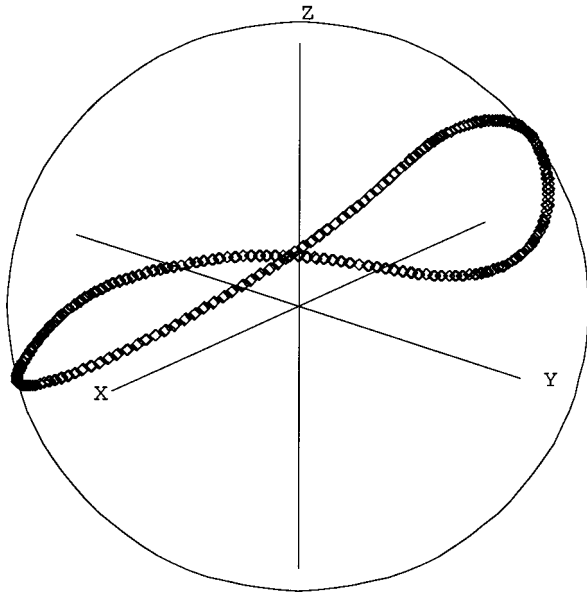


FIG. 7. Poincaré section $X=0$ for the 3:1 resonance, with $E=24.10539$, $B=0.5$, $C=1.0$, $m=16$, showing quasiperiodic motion on the spin sphere.

It is a consequence of the semiquantum equations (6)–(10) that the length of the vector \vec{a} is constant. Therefore, an initially pure state for the spin, interacting with a single classical particle, will always remain pure, and so cannot remain a good approximation to the full quantum theory. This difficulty disappears when it is realized that the classical limit of a quantum state is normally an ensemble of classical trajectories, rather than a single classical trajectory [17,18]. It is, therefore, necessary to construct an ensemble of classical particles whose position and momentum probability distributions agree with those of the initial wave function of the quantum theory. For each member of the ensemble, the vector \vec{a} executes a different orbit on the surface of the unit sphere, and the average of these vectors over the semi-

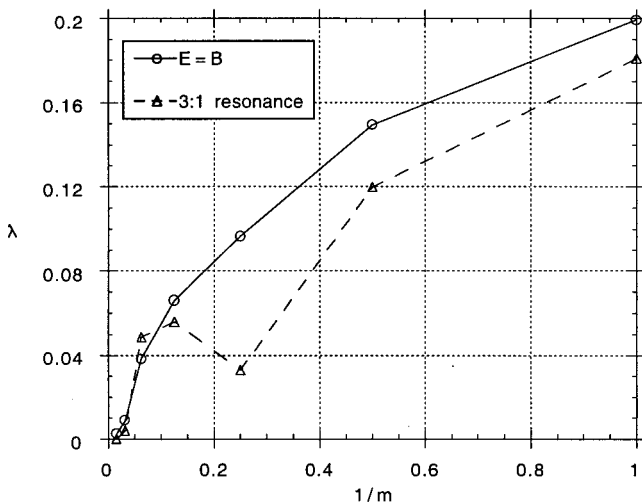


FIG. 8. Largest semiquantum Lyapunov exponent λ vs reciprocal mass.

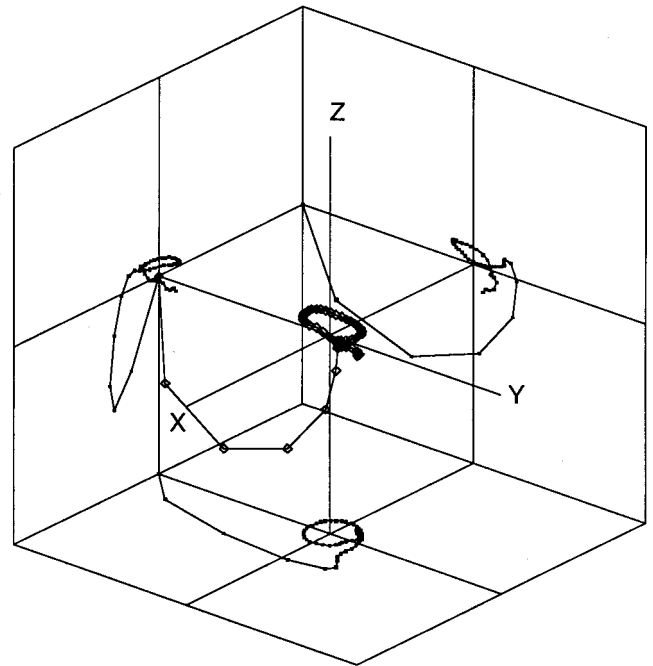


FIG. 9. Spin polarization vector \vec{a} of the full quantum state, and its projections onto the Cartesian planes, for $E=B=0.5$, $C=1.0$, $m=64$. The curve starts at the point $(0, -1, 0)$, and adjacent points are separated by a time interval $\Delta t=0.2$. The X, Y, and Z axes extend from -1 to 1 , with the labels at the positive ends.

quantum ensemble, $\langle \vec{a} \rangle_{\text{sqe}}$, is to be compared with the polarization vector of the full quantum theory (Fig. 10). The depolarization of the semiquantum ensemble matches that due to entanglement of the full quantum state quite well, at least for a limited time.

The difference between the polarization vector of the full quantum theory and the average polarization vector of the semiquantum ensemble is shown in Fig. 11 for mass $m=64$. As a conventional measure of the time during which

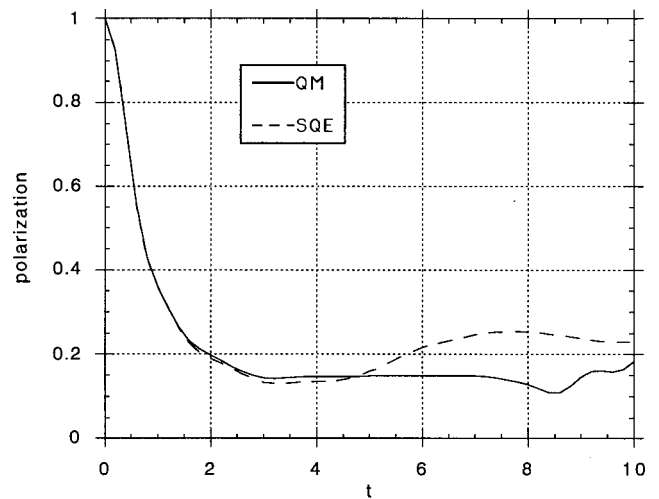


FIG. 10. Magnitude of the polarization vector for the full quantum state (QM) and for the semiquantum ensemble (SQE), for $E=B=0.5$, $C=1.0$, $m=64$.

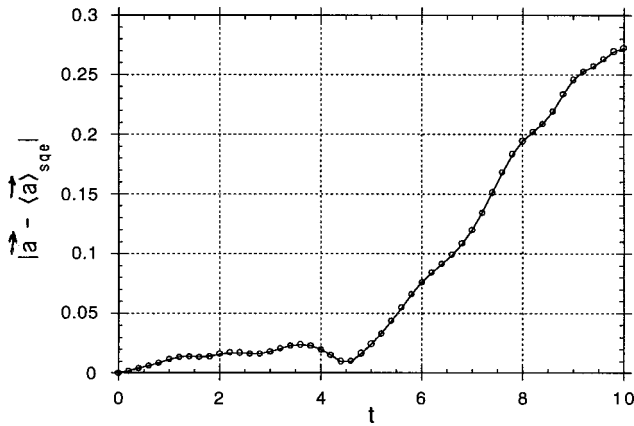


FIG. 11. Difference between the polarization vectors of the full quantum state and of the semiquantum ensemble, for $E=B=0.5$, $C=1.0$, $m=64$.

the semiquantum approximation is accurate, we choose $t_{0.05}$, the time when the difference reaches 0.05. Figure 12 shows that $t_{0.05}$ increases with the mass of the particle, as expected, but only very slowly. It is not closely related to the Lyapunov time, $1/\lambda$, as the latter changes by a factor of 100 while the former changes by only a factor of 10.

V. DISCUSSION

The question posed in the title of this paper has been answered negatively. Semiquantum chaos disappears rapidly as one enters the regime ($m \rightarrow \infty$) where the semiquantum approximation is accurate. One may now ask whether this result, derived for the spin-particle model, is of greater generality. There is good reason to believe that it is more general. The spin could stand for any two-level quantum system. Any nonlinear oscillator will have the property that its natural frequency decreases as its mass is increased at constant energy, hence the argument of Zaslavsky *et al.* [13] for an exponentially narrow chaotic separatrix layer, which was invoked in Sec. III, should also apply. If, on the other hand, the energy of the oscillator is varied to keep the spin and the particle in resonance, then the energy of the oscillator will become very much greater than that of the spin, and the perturbation on the oscillator by spin will become too weak to drive it to chaos. Thus there is good reason to believe that our result will also hold for very many systems comprising a quantum part coupled to a nonlinear oscillator.

If the classical part of the system had more than one degree of freedom, it could be chaotic without coupling to the quantum part. It is, of course, trivial that the state of the quantum system would be driven chaotically by such a chaotic driver. Such systems are excluded from our consideration, since quantum dynamics plays no part in causing that kind of chaos.

The semiquantum approximation improves as the mass of the particle increases. It had previously been suggested [11] that the semiquantum approximation would remain accurate only for a time shorter than the Lyapunov time $1/\lambda$, which would be too short to see the predicted chaos. That is indeed true in our model (see Fig. 12), but mainly because the

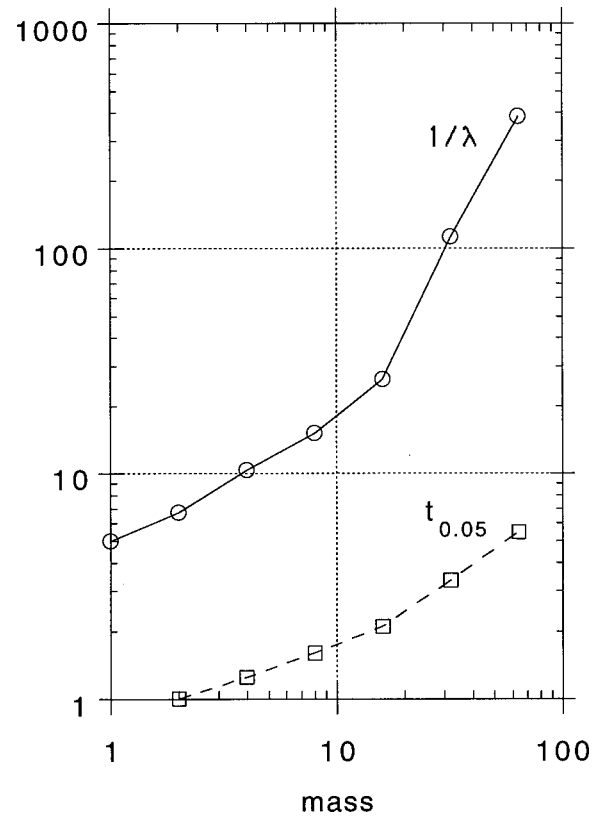


FIG. 12. The Lyapunov time $1/\lambda$ and the break time $t_{0.05}$ (when the polarization-vector difference reaches 0.05) vs mass.

Lyapunov time diverges as λ goes rapidly to zero. But the time during which the semiquantum approximation is accurate ($t_{0.05}$ in Fig. 12) is not closely related to the Lyapunov time. This should not be surprising, since the latter characterizes only the chaotic motions, which cease to exist as $m \rightarrow \infty$.

ACKNOWLEDGMENT

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APPENDIX: CLASSICALITY PARAMETERS

The two dimensionless parameters η and Λ introduced in Sec. II C to describe the degree of classicality of the particle will now be evaluated. Since only orders of magnitude and scaling properties are of interest, we shall omit numerical factors and use the symbol “ \approx ” to denote order-of-magnitude equality. It is convenient to write the potential as $V(x) = Dx^4/4$, where D is a dimensional constant.

The classical action of the particle orbit is $J \approx P_0 X_0$, where P_0 and X_0 are the extents of the phase-space orbit in the momentum and position directions. Their magnitudes are determined by $P_0^2/m \approx E_p$ and $V(X_0) \approx E_p$, where E_p is the particle energy. Thus we have

$$P_0 \approx (mE_p)^{1/2}, \quad X_0 \approx (E_p/D)^{1/4}. \quad (\text{A1})$$

If we take Λ to be the ratio of the quantum of action to the classical action, $\Lambda = \hbar/J$, then we obtain

$$\Lambda \approx \hbar m^{-1/2} E_p^{-3/4} D^{1/4}. \quad (\text{A2})$$

In Sec. II C, Λ was defined to be λ_{DB}/X_0 , the ratio of the deBroglie wavelength to the spatial extent of the orbit. Using $\lambda_{\text{DB}} \approx \hbar/P_0$ and Eqs. (A1), we obtain the same expression (A2) for Λ .

The particle energy levels can be estimated by setting $J \approx n\hbar$, where n is an integer. This yields

$$E_p \approx (n\hbar/\sqrt{m})^{4/3} D^{1/3}. \quad (\text{A3})$$

The level spacing can be approximated by $\Delta E_p = \partial E_p / \partial n$. Using Eq. (A3) to express n in terms of E_p then yields

$$\Delta E_p \approx \hbar m^{-1/2} E_p^{1/4} D^{1/4}. \quad (\text{A4})$$

The spacing between spin energy levels is $\Delta E_s \approx B$, so the ratio of ΔE_p to ΔE_s is

$$\eta \approx \hbar m^{-1/2} E_p^{1/4} D^{1/4} B^{-1}. \quad (\text{A5})$$

Since the potential $V(x)$ has the form of a power law, it is natural to rescale the length x so as to make $D = 1$, as is done in Sec. II C.

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