Inadequacy of Ehrenfest's theorem to characterize the classical regime

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The classical limit of quantum mechanics is usually discussed in terms of Ehrenfest's theorem, which states that, for a sufficiently narrow wave packet, the mean position in the quantum state will follow a classical trajectory. We show, however, that that criterion is neither necessary nor sufficient to identify the classical regime. Generally speaking, the classical limit of a quantum state is not a single classical orbit, but an ensemble of orbits. The failure of the mean position in the quantum state to follow a classical orbit often merely reflects the fact that the centroid of a classical ensemble need not follow a classical orbit. A quantum state may behave essentially classically, even when Ehrenfest's theorem does not apply, if it yields agreement with the results calculated from the Liouville equation for a classical ensemble. We illustrate this fact with examples that include both regular and chaotic classical motions.

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I. EHRENFEST'S THEOREM

It is generally agreed that classical mechanics should emerge from quantum mechanics in some limit. That limit is often loosely described as $\hbar\to 0$, but since the quantum state function depends on $\hbar$ the limit involves a sequence of states that must be defined. This may be done by fixing the values (or distributions) of sufficiently many observables. In many cases, the appropriate limit can be expressed as $\hbar\to 0, n\to\infty$, with $\hbar n$ constant (n is a typical quantum number). That is to say, the quantum $\hbar$ must become small compared to the macroscopic action $\hbar n$. It is not satisfactory to restrict attention to a contrived sequence of wave functions, such as minimum uncertainty packets whose width in both position and momentum varies as $\sqrt{\hbar}$. The classical limit seldom leads to such wave functions. Anticipating the results of this paper, we point out that *the classical limit of a quantum state is an ensemble of classical orbits, not a single classical orbit.* A suitable practical criterion for classical behavior is, therefore, that the quantum averages and probability distributions should agree, approximately, with classical averages and probabilities.

Discussions [1–8] of the classical limit have often been based on Ehrenfest's theorem, which states that, under certain conditions, the centroid of a wave-packet state will follow a classical trajectory.

The essential points of the theorem can be demonstrated with the example of a one-dimensional particle moving in a scalar potential $V(x)$, which generates the force $F(x)=-\nabla V(x)$. Its Hamiltonian operator (we use the circumflex to distinguish operators) is

$$\hat{H}=\hat{p}^2/2m+V(\hat{q}) , \tag{1}$$

and the Heisenberg equations of motion are

$$d\hat{q}/dt=\hat{p}/m , \tag{2}$$

$$d\hat{p}/dt=F(\hat{q}) . \tag{3}$$

Taking the average in some state yields

$$d\langle\hat{q}\rangle/dt=\langle\hat{p}\rangle/m , \tag{4}$$

$$d\langle\hat{p}\rangle/dt=\langle F(\hat{q})\rangle . \tag{5}$$

Now *if* we can approximate the average of the function of position with the function of the average position,

$$\langle F(\hat{q})\rangle\approx F(\langle\hat{q}\rangle) , \tag{6}$$

then (5) may be replaced by (5a):

$$d\langle\hat{p}\rangle/dt=F(\langle\hat{q}\rangle) . \tag{5a}$$

Equations (4) and (5a) then state that the average position and the average momentum in this quantum state will follow a classical trajectory; this is Ehrenfest's theorem. It holds, in particular, if the state function in configuration space is a wave packet whose width is small compared to the scale over which the force $F(x)$ varies appreciably.

In most books the discussion ends at this point, and the impression is given that the above condition defines the classical regime. [Some books [4–8] fail to mention the essential role of the approximation (6), and state, incorrectly, that Eqs. (4) and (5) ensure that the centroid of a wave packet will follow a classical trajectory.] However, we show in this paper that the conditions for the applicability of Ehrenfest's theorem are *neither necessary nor sufficient* to define the classical regime.

Lack of sufficiency is proved by the example of the harmonic oscillator. In that case the force $F(x)$ is a linear function, and so (6) holds as an identity for all states. Yet we know that a quantum harmonic oscillator is not equivalent to a classical harmonic oscillator. In particular, the thermal equilibrium energy, and hence the specific heat, is different for classical and quantum oscillators, and it was this difference that first led Max Planck to introduce the notion of the quantum.

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To demonstrate the lack of necessity, i.e., that a system may violate Ehrenfest's theorem and yet behave essentially classically, is more subtle. We shall illustrate it with several examples.

II. DEVIATIONS FROM EHRENFEST'S THEOREM

Let us introduce operators for the deviations from the mean values:

$$\delta\hat{q} = \hat{q} - \langle \hat{q} \rangle \ , \tag{7}$$

$$\delta\hat{p} = \hat{p} - \langle \hat{p} \rangle \ , \tag{8}$$

and expand (2) and (3) in powers of these operators. Taking the average in some chosen state then yields, in place of (4) and (5),

$$dQ/dt = P/m \ , \tag{9}$$

$$\frac{dP}{dt} = F(Q) + \tfrac{1}{2}\langle (\delta\hat{q})^2 \rangle \frac{\partial^2}{\partial Q^2} F(Q) + \cdots \ , \tag{10}$$

where $P = \langle \hat{p} \rangle$ and $Q = \langle \hat{q} \rangle$. If $\langle (\delta\hat{q})^2 \rangle$ and the higher-order terms are negligible, we recover Ehrenfest's theorem, and Q and P obey the classical equations. It is therefore tempting to interpret the terms involving $(\delta\hat{q})$ as quantum corrections, whose smallness provides the criterion for the classical regime. That interpretation is made in [1–3]; however, it is not correct.

That the terms beyond $F(Q)$ in (10) are not purely quantum mechanical in origin is indicated by the fact that $\langle (\delta\hat{q})^2 \rangle$ does not vanish in the limit of $\hbar \to 0, n \to \infty$, with the total action $\hbar n$ held constant. (Here n is a typical quantum number.) This is easily verified for harmonic-oscillator and hydrogenic eigenstates. In fact, $\langle (\delta\hat{q})^2 \rangle$ is just a measure of the width of the probability distribution in configuration space, which need not vanish in the classical limit. We should, therefore, compare (10) with the statistical form of classical dynamics.

Let $\rho(q,p,t)$ be the probability distribution in phase space for a classical ensemble. It satisfies the Liouville equation

$$\frac{\partial}{\partial t}\rho(q,p,t) = -\frac{p}{m}\frac{\partial}{\partial q}\rho(q,p,t) - F(q)\frac{\partial}{\partial p}\rho(q,p,t) \ . \tag{11}$$

From it, we can calculate the classical averages

$$\langle q \rangle_c = \int\int q\rho(q,p,t)dq\,dp \ , \tag{12}$$

$$\langle p \rangle_c = \int\int p\rho(q,p,t)dq\,dp \ . \tag{13}$$

Differentiating these expressions with respect to t, using (11), and integrating by parts as needed, we obtain

$$d\langle q \rangle_c/dt = \langle p \rangle_c/m \ , \tag{14}$$

$$d\langle p \rangle_c/dt = \int\int F(q)\rho(q,p,t)dq\,dp \ , \tag{15}$$

which are the classical analogs of (4) and (5). Expanding (15) in powers of $\delta q = q - \langle q \rangle_c$ then yields

$$\frac{d}{dt}\langle p \rangle_c = F(\langle q \rangle_c) + \tfrac{1}{2}\langle (\delta q)^2 \rangle_c \frac{\partial^2}{\partial \langle q \rangle_c^2} F(\langle q \rangle_c) + \cdots \ , \tag{16}$$

where $\langle (\delta q)^2 \rangle_c = \int\int (\delta q)^2 \rho(q,p,t)dq\,dp$ is a measure of the width of the classical probability distribution. The significance of the terms involving δq is now clear: the centroid of a classical ensemble need not follow a classical trajectory if the width of the probability distribution is not negligible. Since the quantal equation (10) has exactly the same form as (16), it is apparent that the terms in (10) involving $\delta\hat{q}$ are not to be interpreted as quantum corrections to classical behavior; they merely express the fact that the centroid of the quantum probability distribution does not follow a classical trajectory. Thus the violations of Ehrenfest's theorem, expressed by the higher-order terms of (10), are not necessarily of quantum-mechanical origin; a classical ensemble behaves similarly.

Although (10) and (16) are identical in form to all orders, it does not follow that quantal and classical probability distributions will evolve identically if they are identical at $t=0$. Even their means need not evolve identically. This is so because the time dependence of the mean $\langle q \rangle$ depends, through (9) and (10), on the moments of the distribution, $\langle (\delta q)^n \rangle$, for all positive values of n. The time dependence of the higher moments of the quantum probability distribution can be calculated; the result for $n=2$ is

$$\frac{d}{dt}\langle (\delta\hat{q})^2 \rangle = \langle (\delta\hat{p})(\delta\hat{q}) + (\delta\hat{q})(\delta\hat{p}) \rangle / m \ . \tag{17}$$

The classical expression is similar, except that the order of δq and δp becomes irrelevant. Whereas the quantal (10) agrees with its classical analog (16) provided the classical ensemble is chosen to have the same distributions for q and for p as does the quantum state, the agreement of (17) with its classical analog demands the additional requirement that the classical correlation function $\langle (\delta p)(\delta q) \rangle_c$ should agree with the symmetrized quantum correlation function in (17). As we proceed to higher-order time derivatives, we encounter higher-order correlations involving more and more inequivalent orders of the factors $\delta\hat{p}$ and $\delta\hat{q}$, and it becomes impossible to fit all of them with a single classical phase-space distribution. Thus it is ultimately the noncommutativity of operators $\delta\hat{p}$ and $\delta\hat{q}$ that is responsible for the different evolutions of the classical and quantal probability distributions.

III. PARTICLE BETWEEN REFLECTING WALLS

The similarities and differences between the classical and quantum dynamics can be illustrated by means of a simple example. Consider a particle confined to move between two impenetrable walls, at $x=0$ and L. A general time-dependent state function can be expanded in terms of the energy eigenfunctions

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \sin(k_n x)\exp(-iE_n t/\hbar) \ , \tag{18}$$

where $k_n = n\pi/L$, and $E_n = (\hbar^2\pi^2/2mL^2)n^2$. Because all the frequencies in (18) are integer multiples of the lowest frequency, it follows that $\psi(x,t)$ is periodic, but is period

$$T_{QM} = 4mL^2/\pi\hbar \tag{19}$$

bears no relation to the classical period of a particle with speed v, $T_{cl} = 2L/v$. The failure of (18) to oscillate with the classical period would be a problem if, in the classical limit, the wave function were supposed to describe the orbit of a single particle. But there is no difficulty if it is compared to an ensemble of classical orbits, since the motion of the ensemble need not be periodic. The quantum recurrence period T_{QM} diverges to infinity as $\hbar \to 0$, and so becomes irrelevant in the classical limit.

Let us consider an initial wave function of the form

$$\psi(x,0) = A(x)\exp(ikx) \ , \tag{20}$$

where $A(x)$ is a real amplitude function. The mean velocity of this state is $v = \hbar k/m$. The motion of this quantum state will be compared to that of a classical ensemble whose initial position and momentum distributions are equal to those of the quantum state (2), the initial phase-space distribution being the product of the position and momentum distributions.

As a first example, we take a Gaussian amplitude

$$A(x) = C\exp\{-[(x-x_0)/2a]^2\} \ . \tag{21}$$

This initial state has rms half-width $\Delta x = a$, and its mean position is taken to be $x_0 = L/2$. Results for $a = 0.1, v = 20$ (units: $\hbar = m = L = 1$) are shown in Fig. 1. The average position of the quantum state, $\langle x \rangle = \langle \psi(x,t)|x|\psi(x,t)\rangle$, exhibits a complex pattern of decaying and recurring oscillations that repeat with period T_{QM}. The average position of the classical ensemble closely follows the first quantum oscillations, but it decays to a constant value $\langle x \rangle = L/2$, where it remains. The decay of the classical oscillation is due to the distribution of velocities in the ensemble, which causes it to spread and eventually cover the range $(0,L)$ uniformly. The spreading of the quantum wave function is essentially equivalent to the spreading of the classical ensemble. The later periodic recurrences of the quantum state are due to the interference of reflected waves and to the discreteness of the quantum spectrum, and are essentially nonclassical.

The time interval during which the classical and quantum theories agree well is shown in more detail in Fig. 2. Ehrenfest's theorem, which predicts $\langle x \rangle$ to follow a classical trajectory, is very inaccurate, even before the first reflection. But the failure of Ehrenfest's theorem does not indicate nonclassical behavior; the quantum state and the classical ensemble are in close agreement, even though Ehrenfest's theorem is not applicable. The lower half of Fig. 2 shows that $\Delta x = (\langle x^2 \rangle - \langle x \rangle^2)^{1/2}$ is also correctly given by the classical theory for $t \le 0.14$. The nonmonotonic behavior of Δx is caused by the folding of the ensemble upon itself when it is reflected from a wall. Indeed, for $t = 0.025$ the value of Δx is smaller than it was for the original minimum-uncertainty wave function. For large t, the rms half-width of the classical ensemble

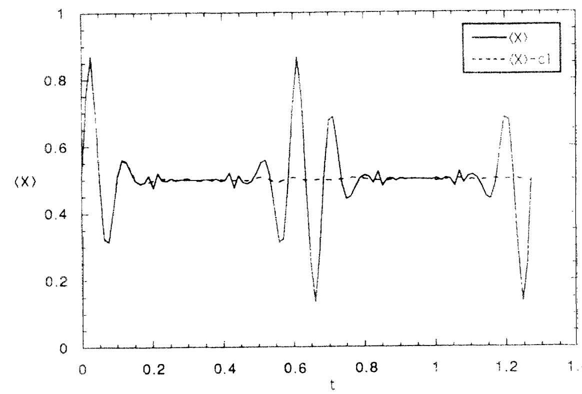

FIG. 1. Average position for a particle confined to the unit interval, according to quantum theory (solid line) and classical ensemble theory (dotted line). The initial state is Gaussian with half-width $a = 0.1$ and mean velocity $v = 20$.

approaches the limit $\Delta x \to L(2\sqrt{3})^{-1} \approx 0.2887L$, which is the value for a uniform distribution.

The close correspondence between classical and quantum theories is not restricted to minimum uncertainty (Gaussian) states. Figure 3 shows results for an (unnormalized) amplitude function of the form

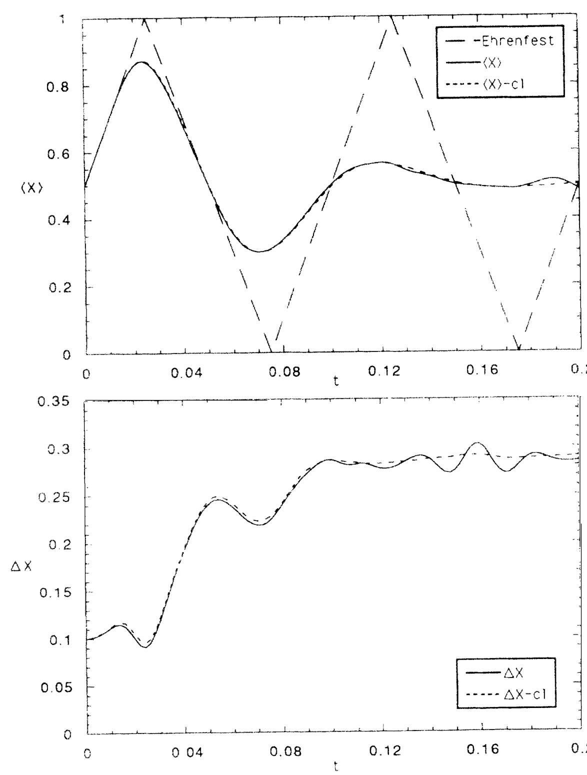

FIG. 2. Upper half: average position according to quantum and classical theories compared with Ehrenfest's theorem (sawtooth curve). Lower half: rms half-width of the position probability distribution, according to quantum (solid line) and classical theories (dotted line).

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\begin{aligned}
A(x) &= (4x)^4 \quad (0 \le x \le \tfrac{1}{4}) \\
&= 2-[4(x-\tfrac{1}{2})]^4 \quad (\tfrac{1}{4} \le x \le \tfrac{3}{4}) \\
&= [4(1-x)]^4 \quad (\tfrac{3}{4} \le x \le 1) \ . \qquad (22)
\end{aligned}
$$

This function and its derivative are continuous, but its quartic behavior near the maximum makes it qualitatively different from a Gaussian. The degree of agreement between the classical and quantum theories is similar to that in Fig. 2.

In this model the large quantum-number limit ($n \to \infty$) is equivalent to the limit of large mean velocity. The damping rate of the oscillations in $\langle x \rangle$ is governed by the width of the velocity distribution in the initial state, and so is unaffected by the limit $n \to \infty$. Thus the time during which the classical oscillations are apparent does not increase with n. But the frequency of the oscillations, and hence the number of oscillations during the damping time, is proportional to n. Thus the classical periodicity becomes better and better defined as $n \to \infty$, even though the wave function (18) never exhibits a true periodicity with the classical period $T_{\rm cl}$.

In the regime where the quantum and classical results agree, the quantum and classical position probability densities are not necessarily the same in detail. In fact, the quantum probability density is approximately equal to the classical density *modulated by an interference pattern,* but the interference pattern is averaged out in calculating $\langle x \rangle$ and $\langle x^2 \rangle$. The classical limit is characterized, not by the absence of interference, but by the interference pattern being too fine to be resolved.

IV. DRIVEN QUARTIC OSCILLATOR

Whereas the previous model was simple and integrable, this model is not integrable. It consists of a quartic anharmonic potential and an external driving force. The Hamiltonian is

$$H = p^2/2m + bx^4 - fx\cos(\omega t) \ . \qquad (23)$$

The parameter values used are $m=1$, $b=0.25$, $f=0.5$, and $\omega=1$. For these parameters, the phase space of the system contains a large island of regular orbits surrounded by a larger zone of chaotic orbits (see Fig. 1 of Ref. [9]). The quantum-mechanical Hamiltonian is obtained from (23) by introducing the momentum operator

$$\hat{p} = -i\hbar\partial/\partial x \ , \qquad (24)$$

with $\hbar=0.02$. This magnitude of $\hbar$ is made more meaningful by comparing it to the area of the regular island in phase space, which is 2.25, and is capable of supporting $2.25/2\pi\hbar = 17.9$ quantum states.

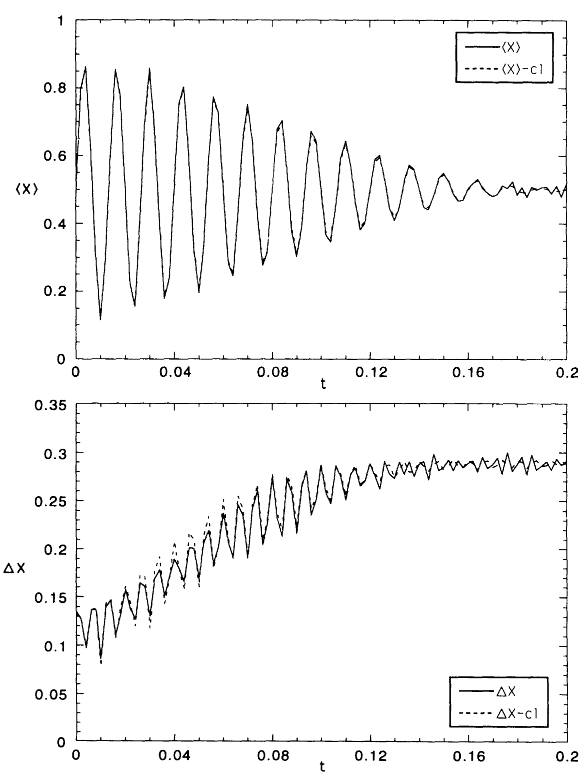

FIG. 3. Average and rms half-width of the position probability distribution for a non-Gaussian state with mean velocity $v=150$, according to quantum (solid line) and classical theories (dotted line).

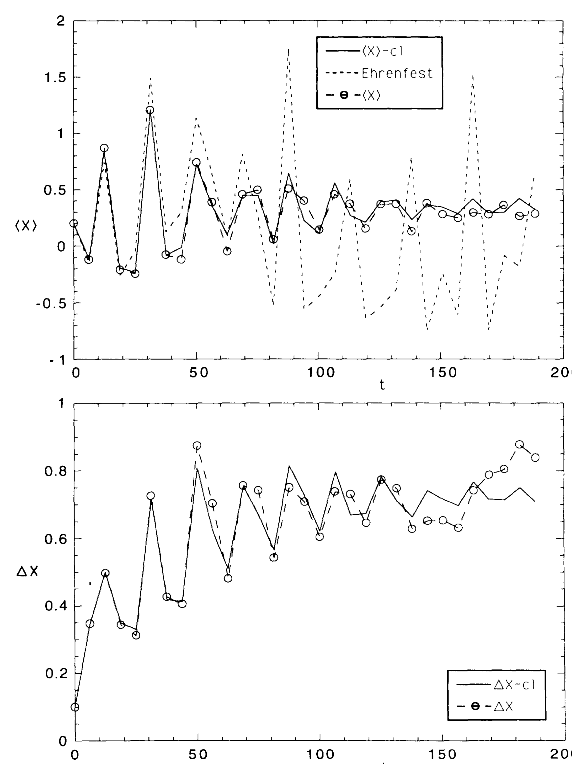

FIG. 4. Driven quartic oscillator in a classically chaotic state. Upper half: average position according to quantum (circles) and classical theories (solid line), compared with Ehrenfest's theorem (dotted line). Lower half: rms half-width of the position probability distribution, according to quantum (circles) and classical theories (solid line).

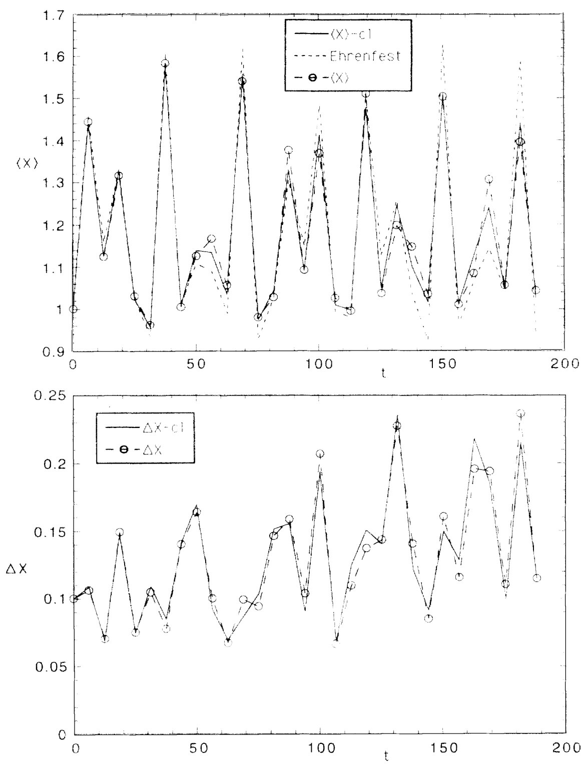

FIG. 5. Driven quartic oscillator in a classically regular state. (Details as in Fig. 4.)

The computations for the classical theory were done by integrating Hamilton's equations for each of the 50 000 particles in the ensemble, using a variable-order variable-time-step Adams method. For the quantum theory, we used a spatial finite-difference discretization of the time-dependent Schrödinger equation, with 3000 grid points in the range $-2.5 \le x \le 2.5$. This yields a large set of coupled ordinary differential equations, which was integrated with a Runge-Kutta-Merson routine.

The initial (quantum and classical) states were chosen to be Gaussians, as described in Sec. III, with $\Delta x = \Delta p = 0.1$. The results of Fig. 4 were obtained by placing the centroid of the initial state in the chaotic zone, at $\langle x \rangle = 0.2, \langle p \rangle = 0$; those of Fig. 5 were obtained by placing the centroid in the regular island, at $\langle x \rangle = 1.0, \langle p \rangle = 1.0$. In Figs. 4 and 5, the data points are plotted at times $t = 2\pi n/\omega$ for integer n, and so the results shown correspond to a stroboscopic plot (Poincare section). The detailed oscillations of $\langle x \rangle$ and Δx within one period of the driving force are not shown because that amount of detail would make the figures confusingly complex.

As expected, the half-width Δx of the state grows much more rapidly in the chaotic case than in the regular case, and, as a result, Ehrenfest's theorem breaks down much sooner. But it would be incorrect to conclude from this fact that the classical theory must break down sooner in the chaotic case. In fact, the quantum state and the classical ensemble agree well up to about $t = 140$, long after Ehrenfest's theorem has ceased to apply in the chaotic case. The agreement between classical and quantum theories seems to persist somewhat longer in the regular case, but this is probably due to the fact that the regular motions are confined within the regular island, whereas the chaotic motions can explore a much larger region of phase space. Hence the maximum possible difference is greater for the chaotic case.

V. CONCLUSION

We have shown that Ehrenfest's theorem is *neither necessary nor sufficient* to characterize the classical regime in quantum theory. Ehrenfest's theorem asserts that, for a sufficiently narrow probability distribution, the mean position in the quantum state will follow a classical trajectory. However, generally speaking, the classical limit of a quantum state is not a single classical trajectory, but an ensemble of trajectories [10]. The averages and higher moments of the quantum and classical probability distributions often agree in situations where Ehrenfest's theorem is not applicable. Therefore Ehrenfest's theorem does not define the conditions for classical behavior.

Our conclusion is of more than merely pedagogical significance. The definition of the classical regime is of considerable importance in the study of quantum chaos. In that context, Goggin, Sundaram, and M. Ionni [11] have derived an expansion that expresses a quantum commutator in terms of a classical Poisson bracket plus corrections analogous to those in our (10). They interpret those correction terms as quantum corrections, and assert that the classical limit is obtained *only* if those terms all vanish. But we have shown that some of those corrections have a classical interpretation, and do not vanish in the limit $\hbar \to 0$. In a similar context, Lan and Fox [12] assert that in the classical limit the mean values should follow Hamilton's equations and the rms deviations should be negligible. We have shown that to be an inappropriate criterion to identify the classical limit, and it can be expected to yield inaccurate estimates of the classical regime. In particular, we have shown by an example that, although Ehrenfest's theorem does indeed break down much sooner for chaotic motions than for regular motions, the degree of agreement between the classical ensemble and the quantum state is comparable for both chaotic and regular domains.

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