Quantum-Classical Transition in Nonlinear Dynamical Systems

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Viewed as approximations to quantum mechanics, classical evolutions can violate the positive semidefiniteness of the density matrix. The nature of the violation suggests a classification of dynamical systems based on classical-quantum correspondence; we show that this can be used to identify when environmental interaction (decoherence) will be unsuccessful in inducing the quantum-classical transition. In particular, the late-time Wigner function can become positive without any corresponding approach to classical dynamics. In the light of these results, we emphasize key issues relevant for experiments studying the quantum-classical transition.

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In recent years much effort has been expended, both theoretically and experimentally, to explore the transition from quantum to classical behavior in a controlled way. In this context, the interaction of trapped, cold atoms with optical potentials, both time-dependent and independent, has become a topic of considerable interest and activity [1,2]. Systematic experimental investigation of dissipative quantum dynamics of nonlinear systems is an exciting new area where the frontier between classical and quantum mechanics may be carefully examined.

In this Letter we explore some of the key qualitative features of the quantum-classical transition. We establish that with $\hbar$ fixed at a finite value, and classical dynamical evolution equations for phase space distribution functions viewed as approximations to the underlying quantum equations, classical Liouville and master equations violate the quantum constraint of positive semidefiniteness of the density matrix: We refer to this property of the density matrix as "rho-positivity." We argue that rho-positivity violation can (i) serve to classify dynamical systems with regard to weak and strong violation of classical-quantum correspondence and (ii) explain robustness to decoherence in the sense of avoidance of the expected classical limit as exemplified by dynamical localization in the (open-system) quantum delta kicked rotor (QDKR). Our results impact directly on the interpretation and design of experiments to test various aspects of the quantum-classical transition.

The singular nature of the classical limit $\hbar \to 0$ in quantum mechanics has been appreciated for a long time. However, what has not been stressed sufficiently is the reason for this singular behavior: that classical dynamics violates unitarity and rho-positivity; thus $\hbar = 0$ cannot be connected smoothly to $\hbar \to 0$. A simple argument suffices to make this point clear. Consider as initial condition a pure Gaussian state. Suppose we evolve the corresponding (positive) Wigner function classically in any nonlinear potential (for linear systems classical and quantum dynamics are identical [3]), then the distribution becomes no longer Gaussian, but is still positive definite. Three possibilities now present themselves: the evolved object can be interpreted as (i) a pure quantum state (unitarity is preserved), (ii) a mixed quantum state (rho-positivity is preserved), and (iii) it cannot be interpreted as a quantum state (rho-positivity is violated). The first possibility can be dismissed using Hudson's theorem: the *only* pure state with positive Wigner function is a Gaussian state with a (necessarily) Gaussian-Wigner function [4]. But our distribution is non-Gaussian. As to the second, we first note that the phase space integral of any function of the phase space distribution is preserved under a Liouville flow. In particular, $\int f^2(x,p)\,dx\,dp$ remains constant. For Wigner functions this quantity is proportional to $\mathrm{Tr}\rho^2$ which is a direct measure of whether a state is mixed or not—since this measure cannot change, the evolved object is not interpretable as a mixed state. Thus we are forced to the third alternative, that the evolved object cannot be interpreted as a quantum state at all: the Weyl transform of the evolved classical distribution yields a "classical density matrix" which is non-rho-positive [5], i.e., possesses negative eigenvalues.

In contrast to the idealized *closed* dynamical systems just analyzed, all real experiments deal with *open* systems, i.e., systems interacting with their environment, of which the particular case of an observed system interacting with a measuring apparatus is an important example. In such systems, the object of interest is often a reduced density matrix for the system, obtained by tracing over the degrees of freedom in the environment. The evolution of such a reduced density matrix is given by a master equation which evolves pure states into mixed states and suppresses quantum interference phenomena due to the averaging effect inherent in ignoring the environment variables: This process is termed decoherence. Can the classical analogs of open quantum evolution also be strongly non-rho-positive as in the case of closed systems discussed above? We demonstrate below that the answer is yes.

A quantum master equation representing a weakly coupled, high temperature environment often utilized in studies of decoherence is

$$\frac{\partial}{\partial t} f_W = L_{cl} f_W + L_q f_W + D \frac{\partial^2}{\partial p^2} f_W ; \tag{1}$$

$$L_{cl} \equiv -\frac{p}{m}\frac{\partial}{\partial x} + \frac{\partial V}{\partial x}\frac{\partial}{\partial p}, \tag{2}$$

$$L_q \equiv \sum_{\lambda\,\mathrm{odd}=3}^{\infty} \frac{1}{\lambda!}\left(\frac{\hbar}{2i}\right)^{\lambda-1} \frac{\partial^\lambda V(x)}{\partial x^\lambda}\frac{\partial^\lambda}{\partial p^\lambda}. \tag{3}$$

This master equation also arises when modeling continuous measurement of position [6].

When the diffusion constant $D = 0$, Eq. (1) is the quantum Liouville equation for the closed system. The linearity of the quantum Liouville equation implies that in order for the evolution to be unitary, L_q cannot be unitary since L_{cl} is not (the sum $L_{cl} + L_q$ is unitary but not the operators separately). The familiar heuristic argument for obtaining the classical behavior from the quantum master equation is that the diffusion term smooths out the interference effects generated by L_q in such a way that quantum corrections to the classical dynamics are much reduced. It has also been argued that, at finite $\hbar$, the limiting case of the quantum master equation is in fact the classical Fokker-Planck equation [setting $L_q = 0$ in Eq. (1)] rather than the classical Liouville equation [7]. In any case, one immediately appreciates that if *either of the classical equations is strongly rho-positivity-violating,* then this implies the existence of compensatory "large" quantum corrections in the quantum master equation, and hence the above heuristic argument must fail: L_q is responsible for more than just the generation of interference fringes in the Wigner evolution.

As described below, a particular example of how L_q continues to be important even in the presence of a strongly decohering environment is provided by the stability of certain nonclassical aspects of the dynamics of the QDKR to dephasing effects of external noise and decoherence due to spontaneous emission. Two alternatives exist to explain this stability: (i) diffusion in the quantum master equation is simply not efficient at suppressing quantum interference terms present in the Wigner function or (ii) the much more intriguing possibility that the diffusion is successful in suppressing the interference terms and the Wigner function is (almost) everywhere positive, yet the late-time distribution is not the solution of the corresponding classical Fokker-Planck equation. The second possibility is the one actually realized, and it arises precisely as a consequence of the fact that the classical Fokker-Planck equation strongly violates rho-positivity, while the quantum master equation does not.

We now briefly describe the dynamical systems investigated in detail in this Letter. Previous work has already identified two qualitatively very different behaviors in the dynamics of *closed* quantum systems with regard to the classical-quantum correspondence: (i) Systems exist in which quantum expectation values and classical averages track each other relatively closely as a function of time [7,8], e.g., the driven Duffing oscillator with Hamiltonian,

$$H_{\mathrm{duff}} = p^2/2m + Bx^4 - Ax^2 + \Lambda x \cos(\omega t), \tag{4}$$

and (ii) systems in which the quantum and classical averages diverge sharply after some finite time, e.g., dynamical localization in the QDKR [9]. The Hamiltonian for the delta kicked rotor (DKR) is

$$H_{\mathrm{dkr}} = \frac{1}{2} p^2 + \kappa \cos q \sum_n \delta(t - n). \tag{5}$$

In order to investigate the open-system dynamics for these Hamiltonians, we solved the classical and quantum master equations corresponding to Eqs. (4) and (5) using a high-resolution spectral solver implemented on parallel supercomputers. The solver explicitly respects rho-positivity conservation.

It is important to note that for open systems there always exists a parameter regime in which they effectively follow a classical evolution, not only at the level of expectation values but also in terms of the existence of classical trajectories [10,11]. The existence of such trajectories requires the treatment of observation of the system by the continuous extraction of information from the environment as distinct from simply averaging over it. (Environmental decoherence by itself cannot extract localized "trajectories" from the quantum dynamics.) As established in Ref. [10], quantum-classical correspondence at the level of trajectories occurs only when certain conditions are met. Broadly speaking, these conditions require that the measurement be sufficiently accurate (a localization condition) and that the system action be sufficiently large in units of $\hbar$. Once classical trajectories are generated by the observed quantum dynamics, it follows that quantum and classical averages also must agree. If the conditions of Ref. [10] are satisfied for any two quantum evolutions, the two Hamiltonians can no longer be distinguished based on quantum-classical correspondence. Thus closed-system behavior does not automatically allow one to classify open systems. In this Letter, we specifically concern ourselves with systems in which the conditions are not satisfied. In this more general case, just as for closed systems, there can still be Hamiltonians for which quantum-classical correspondence exists at the level of expectation values (established for the Duffing oscillator in Ref. [7]) and Hamiltonians for which it is violated (the QDKR being a well-known example). These two systems will be shown below to provide examples of weak (Duffing) and strong (DKR) violation of rho-positivity.

We verified that in both the DKR and the Duffing oscillator examples discussed below, the localization condition [10] necessary to obtain classical trajectories was violated. Numerical simulations were used to directly confirm that localized quantum trajectories did not exist in either case. As discussed above, a meaningful distinction between the two sorts of possible evolutions, i.e., strong vs weak violation of correspondence, now becomes possible. As the value of $\hbar$ is reduced (with D fixed and nonzero) one does expect an approach to the classical limit [10], though the trajectory in the space of D and $\hbar$ need not be simple [12].

Our numerical code returns us the classical distribution function, the quantum density matrix, and the Wigner function as functions of time. We then numerically solve for the eigenvalues of the quantum density matrix and the eigenvalues of the Weyl transform of the classical phase space distribution (the "classical density matrix"). Results of one such computation are displayed in Fig. 1 for the DKR and Duffing systems. For the DKR, initial conditions are pure Gaussian-Wigner functions characterized by the standard deviations $\Delta x = 2.5$ and $\Delta p = 1$ (with $\Delta x \Delta p = \hbar/2$), centered on the point $(x, p) = (0, 0)$, and with $\hbar = 5$, $\kappa = 10$, and $D = 0.1$. The horizontal axis refers to the index i corresponding to the eigenvalues λ_i, which are themselves plotted on the vertical axis. The solid line is a result from a numerical solution of the quantum master equation. As expected all eigenvalues are positive (the pure initial state has one eigenvalue equaling unity, the rest being zero). The dashed line is the corresponding result from the classical Fokker-Planck equation, which is characterized by a strong contribution from negative eigenvalues. It is thus clear that the true quantum density matrix and that provided by the classical approximation are in fact quite different. In contrast, results from classical Duffing calculations show a very small contribution from negative eigenvalues. [Parameter values in the particular case shown in Fig. 1 were $m = 1$, $A = 10$, $B = 0.5$, $\Lambda = 10$, $\omega = 6.07$, $\Delta x = 0.05$, $\Delta p = 1$, $(x, p) = (-3, 8)$, $\hbar = 0.1$, $D = 0.02$.] These results show how rho-positivity violation may be used to distinguish the two types of dynamical systems. An important point to emphasize is that it is sufficient to carry out only the classical dynamical calculation in order to check if a dynamical system strongly or weakly violates quantum-classical correspondence. (The initial condition must of course be a Wigner function.) Also, it should be clear that nonviolation of rho-positivity is a necessary but not sufficient condition for quantum-classical correspondence in terms of agreement of expectation values.

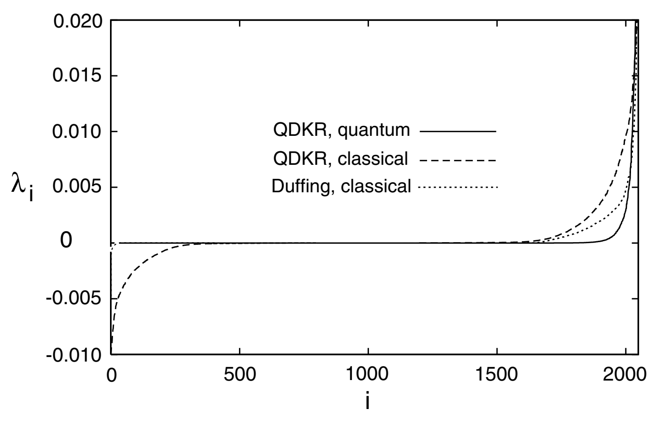

FIG. 1. Eigenvalues of the quantum density matrix (solid line) and the classical approximation (long-dashed line) computed from the quantum and classical master equation evolutions for the DKR at $t = 6$. Also shown (short-dashed line) is the classical result for the Duffing oscillator at $t = 10$.

It is well known that dynamical localization in the QDKR can be destroyed (in the sense that $\langle p^2(t) \rangle$ no longer saturates at late times) by coupling to external noise or to dissipative channels (e.g., spontaneous emission) [13]. However, even in the presence of quite strong coupling to these decohering channels, the evolution does not go over to the classical one, and in this sense the DKR is quite different from the Duffing system investigated in Ref. [7]. While in this Letter we considered a simple form of environmental interaction (1), we have checked that including amplitude and phase noise, timing jitter in the kicked system, and spontaneous emission does not change the generic behavior. (A detailed investigation of the DKR in a realistic experimental configuration may be found in Ref. [14].) Since we know that the DKR strongly violates correspondence (Fig. 1), this behavior is essentially forced: as long as the classical evolution strongly violates rho-positivity, it is impossible for the full evolution to ever become close to the classical one as the quantum corrections must always be concomitantly large. However, an interesting question still remains as to whether the resulting Wigner function at least has a classical interpretation. In order to investigate this we computed as a function of time the quantity $\Gamma = \int dx\, dp\, (|f_W| - f_W)$, which provides a global measure of negativity of the Wigner function. The results are displayed in Fig. 2. With $D = 0$, one sees that Γ increases monotonically as the Wigner function develops the expected oscillatory structure as a consequence of quantum interference in phase space. When $D \neq 0$, diffusion in phase space wipes out the interference and produces an essentially positive distribution which one may interpret classically. However, because rho-positivity must be maintained, classical evolution cannot connect two such positive distributions. Thus, in systems where

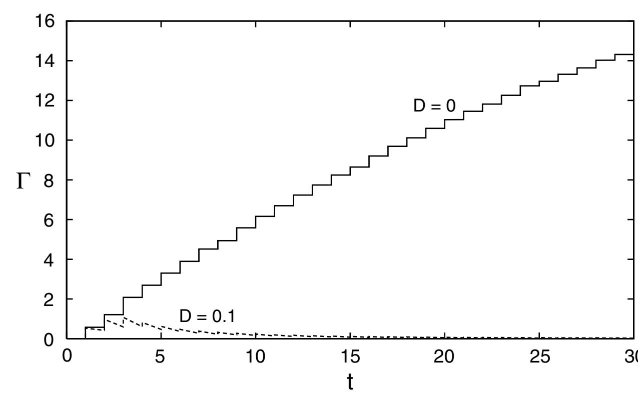

FIG. 2. The Wigner function negativity measure Γ as a function of time for $D = 0$ and $D = 0.1$ for the QDKR.

correspondence is strongly violated, decoherence can be successful in rendering the Wigner distribution positive, but yet not lead to the expected classical limit. We note that in NMR systems an interesting question arises as to whether a classical evolution of a spin ensemble can reproduce results from a quantum evolution connecting initial and final ensemble spin states that are both unentangled (and thus may be interpreted as classical distributions) [15]. We have shown that a similar situation can exist even in single-particle evolution where entanglement is not an issue.

Recent experiments have attempted to directly address the issue of environment-induced decoherence in the QDKR in the context of cold atom optics [1]. Despite some complications stemming from nonideal realizations, the results indicate that classical and quantum evolutions agree only at inordinately large noise levels. In these experiments, parametric noise or spontaneous emission was used as the decohering mechanism. (The nonselective master equation for atomic motion in far-detuned laser light has a similar form to that of a particle subjected to continuous position measurement. However, arguments can be made that only the weak decoherence regime can be accessed in this manner.) The parameter values in our numerical work are close to those actually used in the experiments. Thus, as with our simulations, the experiments are not carried out in a classical regime in the sense of Ref. [10]. Given the strong violation of correspondence inherent in the dynamics of the DKR, it follows immediately that to observe true classical behavior, either the current experiments have to switch to a system which violates correspondence weakly or have to employ smaller values of $\hbar$.

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