Quantum entropy dynamics for chaotic systems beyond the classical limit

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The entropy production rate for an open quantum system with a classically chaotic limit has been previously argued to be independent of $\hbar$ and D, the parameter denoting coupling to the environment, and to be equal to the sum of generalized Lyapunov exponents, with these results applying in the near-classical regime. We present results for a specific system going well beyond earlier work, considering how these dynamics are altered for the Duffing problem by changing $\hbar, D$ and show that the entropy dynamics have a transition from classical to quantum behavior that scales, at least for a finite time, as a function of $\hbar^2/D$.

Consider a quantum system with a nonlinear classical limit: Nonclassical effects depend on the size of Planck's constant $\hbar$ compared to the characteristic action. Further, the system-environment interaction as measured through some parameter D, is crucial [1]. The dynamics of the classical limit of the problem are important [2] particularly through the classical Lyapunov exponents λ. It has recently been found that the quantum entanglement rate for chaotic systems shows a valuable speed-up [3] but this is to be balanced against the observed enhanced decoherence effects for chaotic systems in the classical limit [4–6]. However, there is increased stability against fidelity decay deep in the quantum parameter regime [7], leading to the proposal to "chaoticize" quantum computation [8]. This complex multiparameter quantum-classical transition is fundamental, poorly understood, and also valuable in understanding the behavior of quantum devices.

A recent analysis [9], summarized below, suggested that headway could be made in characterizing the full range of behavior by considering composite parameters and scaling. That is, the quantum-classical difference as measured by some quantity $QC_d(\hbar, D, \lambda)$ should be the simpler function $QC'_d(\zeta)$ of a single composite parameter $\zeta = \hbar^\alpha D^\beta \lambda^\gamma$. Evidence has begun to accumulate [10] supporting this perspective. These come mostly from studying the effect of changing $D, \hbar$ on time-independent (usually from $t \to \infty$) measures QC_d. The change with λ is harder to study since the classical phase-space changes along with λ. A different but related issue is the nonequilibrium statistical mechanics of a nonlinear quantum system as measured through the system's entropy dynamics. A powerful result of broad interest is that the entropy production rate for an open quantum system with a classically chaotic limit is independent of $\hbar$ and D and is equal to the sum of generalized Lyapunov exponents [4–6]. However, this has been verified only in the classical limit, and despite the considerable interest in this, there are few useful results away from this limit.

In this paper, we start with the argument that quantum-classical distance can be measured sensibly with a quantum system's linear entropy. We then study the entropy dynamics for the chaotic Duffing oscillator as a function of $\hbar, D$ to obtain several results that considerably extend results on entropy decay as well as generalize the scaling results. Specifically, the Lyapunov exponent dependence is shown to be valid only for a small parameter range and for times. We look, more usefully, at the time-dependent entropy itself which unexpectedly shows scaling with a single parameter $\zeta_0 = \hbar^2/D$, thus generalizing previous results from time-independent measures [9,10]. That is, behavior from widely varied $\hbar, D$ collapse onto curves that depend only on ζ_0, which we explain on the basis of an expansion in ζ_0, as well as direct comparison of dynamics. This enables the characterization of entropy dynamics over a much wider range of parameters and times than previously attempted. We show dynamical regimes which we term (I) classical, (II) semiclassical, and (III) quantum, with a smooth transition between these regimes with increasing ζ_0.

We begin with the master equation for the evolution of a quantum Wigner quasiprobability ρ_W under Hamiltonian flow with potential $V(q)$ while coupled to an external environment [4]:

$$\frac{\partial \rho_W}{\partial t} = L_c + L_q + T \tag{1}$$

$$
\begin{aligned}
= \{H, \rho_W\} &+ \sum_{n \geq 1} \frac{\hbar^{2n}(-1)^n}{2^{2n}(2n+1)!} \frac{\partial^{2n+1} V(q)}{\partial q^{2n+1}} \frac{\partial^{2n+1} \rho_W}{\partial p^{2n+1}} \\
&+ 2\gamma \partial_p(p\rho_W) + D\partial_p^2 \rho_W.
\end{aligned}
\tag{2}
$$

The first term, the Poisson bracket L_c, generates the classical evolution for ρ_W. The terms in $\hbar$ are the quantal "correction" terms (denoted L_q). The environmental coupling (T) is modeled by the diffusive D term and the dissipative γ term. We assume, as typical, short time scales or high temperatures such that the γ term is negligible. A QC_d can then be considered by propagating the same initial condition with $L_q + L_c + T$, compared to using only L_c, or more appropriately using $L_c + T$ from above.

If QC_d is the difference between the expectation values of an observable, it becomes strongly dependent on the observable. For example, even when the centroids of a quantum and classical distribution are behaving identically, differences exist in higher-order moments. Further, measures such as the time when the QC_d hits a predefined value introduce subjectivity. Moreover, while powerful in the abstract, it is

inherently unphysical to propagate something both classically and quantally. Some of these problems can be avoided by monitoring the quantum entropy, which does not measure distances but directly addresses relevant issues of information. The linear or Renyi entropy of second order S_2 is also the natural logarithm of the purity P as $S_2 = \ln(P)$ $= \ln[\text{Tr}\{\hat{\rho}^2\}]$. Note that $P = 2\pi\hbar \, \text{Tr}\{\rho_W^2\}$ where the Tr now represents integration over all phase-space variables. This has been extensively studied and for a system with a classically chaotic limit, it has been argued [4,6] that in the weak-noise, small-$\hbar$ classical limit, $-dS_2/dt$ equals the sum of the positive classical Lyapunov exponents. More careful considerations generalize this to a weighted sum over Lyapunov exponents [5]. For the classical limit itself, this should arguably be further generalized to time-dependent versions [11]. That is, although the previous results apply in some limits or special cases, even the classical behavior is not fully understood. Less is known about the quantum system, particularly the impact of changing scale or noise through $\hbar, D$, which is what we address below. We work with the Hamiltonian H $= \frac{p^2}{2m} - Bx^2 + \frac{C}{2}x^4 + Ax\cos(\omega t)$. This is the Duffing oscillator, which as a one-dimensional driven problem with a quartic nonlinearity is one of the simplest flows with a rich phase-space structure and hence is a paradigmatic problem in Hamiltonian chaos. The quantum version has also been frequently studied, including decoherence issues [6,12].

We briefly review the behavior of the classical density ρ_c in the limit of only the $L_c + T$ evolution. As a result of chaos due to L_c alone, ρ_c increases the fine-scale structure exponentially rapidly, with a rate given by a generalized Lyapunov exponent. When the structure gets to sufficiently fine scales, the noise T becomes important, and it acts to decrease, or coarse-grain, fine-scale structure. These competing effects can be profitably studied using the measure

$$\chi^2 \equiv -\frac{\text{Tr}[\rho_c \nabla^2 \rho_c]}{\text{Tr}[(\rho_c)^2]} = \frac{\text{Tr}[|\nabla \rho_c|^2]}{\text{Tr}[(\rho_c)^2]}, \qquad (3)$$

where χ^2 is approximately the mean-square radius of the Fourier transform of ρ, measuring the structure in the distribution [13]. Most importantly, Eq. (2) yields the identity $dS_2/dt = -2D\chi^2$ [6,14] with this valid classically or quantum mechanically, that is, with both S_2, χ^2 computed for ρ_c or ρ_W [5], respectively. For a classically uniformly chaotic system, the dynamics of χ^2 can be written approximately [15] as a competition between chaos and diffusion as

$$\frac{d\chi^2}{dt} \approx 2\Lambda\chi^2 - 4D\chi^4. \qquad (4)$$

This implies that χ^2 settles after a transient to the metastable (that is, constant for finite-time) value

$$\chi^{2*} = \Lambda/2D, \qquad (5)$$

where Λ is a ρ dependent generalized Lyapunov exponent [15,16]. This *classical* argument leads to the argument [4–6] that quantum entropy-production rates are equal to generalized Lyapunov exponents. This applies to a greater range of parameters than might be anticipated because decoherence suppresses quantum effects. While this behavior has been
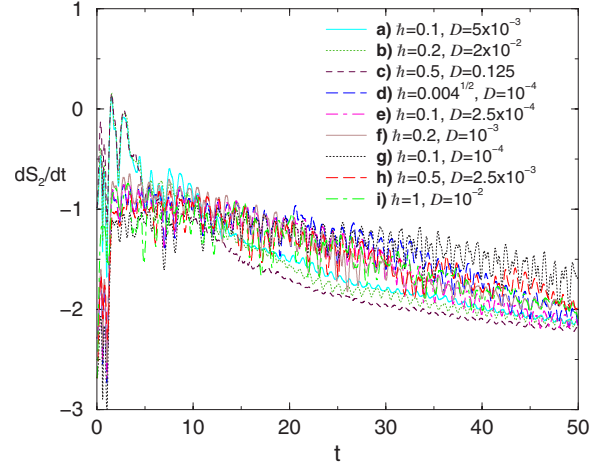

FIG. 1. (Color online) Entropy production rate $\dot{S}_2$ [where S_2 $= \ln(P)$ for states with purity P] for the quantum Duffing oscillator with $m = 1$, $B = 10$, $C = 1$, $A = 1$, $\omega = 5.35$, and $\hbar, D$ as indicated, showing a wide variation in behavior. The initial conditions are Gaussians in the chaotic region with $\langle x \rangle_{t=0} = 1.0$, the spread $\sigma_x^2 = 0.05$, $\langle p \rangle_{t=0} = 0.0$, and the spread σ_p^2 is set by the constraint of defining a minimum-uncertainty state and hence by the particular value of $\hbar$.

shown in several instances, it does not capture the complete picture, particularly the effect of changing $\hbar, D$. We show this in Fig. 1 plotting dS_2/dt for the Duffing problem with $m = 1$, $B = 10$, $C = 1$, $A = 1$, $\omega = 5.35$, as previously used [6]. The behavior, over a wide parameter and time range, is quite complicated. If a subset (all of those with $\hbar = 0.1$) are plotted for a short time ($t < 15$) as in [6], they show the classical Lyapunov exponent entropy-production behavior [4–6]. This is valid only for some small range of parameters and short times. There has been a suggestion of a superposition of classical and quantal exponential decay [17] for the purity. This would lead to a crossover transition within a fairly narrow range from one constant value to another in Fig. 1, which we do not see. Other ways of considering the data (as in Fig. 2 below) also do not support this. In general the search for these small regimes of linear decay for entropy is not as helpful as understanding the broader parameter dependence.

To do this, consider as in Fig. 2, $\text{Tr}\{\rho_W^2(t)\}/\text{Tr}\{\rho_W^2(0)\}$. Since the y axis is logarithmic, we are effectively looking at $\ln(\text{Tr}\{\rho_W^2(t)\}) - \ln(\text{Tr}\{\rho_W^2(0)\}) = S_2(t) - S_2(0) = S(t)$ for our pure-state Gaussians. This shows useful organization invisible in Fig. 1 due to the small-scale variation in a narrow range. Most interestingly, the entropy dynamics for the wide variety of parameters considered is captured entirely for the times shown by the composite parameter $\hbar^2/D \equiv \zeta_0$, even though a wide range of behavior, not obviously characterized as exponential decay, is seen as ζ_0 is varied. Larger ζ_0 corresponds to high $\hbar$ or low noise D or both, and remains closer to a pure quantum state for longer times, which makes physical sense. Note also that there is some ζ_0 dependence for the time scale of scaling, with a long-term separation of curves.

We understand this ζ_0 dependence by considering quantum corrections to the classical dynamics, which depend [see
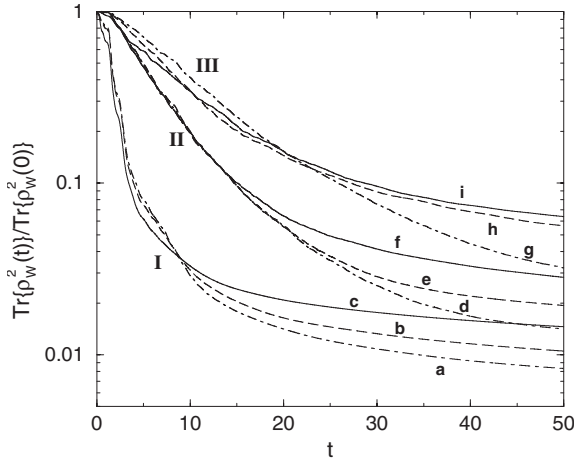
FIG. 2. Evolution of the normalized purity for the same states as Fig. 1 in the quantum Duffing oscillator. Scaling is observed relative to the parameter $\zeta_0 \equiv \hbar^2/D$. (I) Classical: $\zeta_0 = 2$, (a) $\hbar = 0.1$, $D = 5 \times 10^{-4}$, (b) $\hbar = 0.2$, $D = 2 \times 10^{-2}$, and (c) $\hbar = 0.5$, $D = 0.125$. (II) Semi-classical: $\zeta_0 = 40$, (d) $\hbar = 0.004^{1/2}$, $D = 10^{-4}$, (e) $\hbar = 0.1$, $D = 2.5 \times 10^{-4}$, and (f) $\hbar = 0.2$, $D = 10^{-3}$. (III) Quantum: $\zeta_0 = 100$, (g) $\hbar = 0.1$, $D = 10^{-4}$, (h) $\hbar = 0.5$, $D = 2.5 \times 10^{-3}$, and (i) $\hbar = 1$, $D = 10^{-2}$.

Eq. (2)] on the derivatives of the Wigner function. Given that the second derivatives $\partial^2 \rho_W \propto \chi^2$, these corrections scale as

$$L_q \approx \hbar^{2n} \frac{\partial^{2n+1} V(q)}{\partial q^{2n+1}} \frac{\partial^{2n+1} \rho_W}{\partial p^{2n+1}} \approx \hbar^{2n} \chi^{2n+1} V^{(2n+1)}(x), \quad (6)$$

where $V^{(r)}$ denotes the rth derivative of V. When the phase-space distribution hits a metastable state such that χ^2 settles to the fixed value $\Lambda/2D$, the difference between the quantum and classical evolution may be estimated to depend on

$$\zeta \equiv \hbar^{2n} \Lambda^{n+1/2} D^{-(n+1/2)} V^{(2n+1)}(x), \quad (7)$$

where, since χ is a "length" in Fourier space, we have that $x \approx \chi^{-1} = \sqrt{2D/\Lambda}$. This is essentially the same result as that derived in Ref. [12] from a completely different perspective and is also the root of the suggestion in Ref. [9] to search for scaling. Therefore the first order quantum corrections in a semiclassical regime should scale, in complete generality, with the single parameter ζ. The particular form of ζ is decided by the details of the Hamiltonian and the difference between the quantal and classical propagators. For the Duffing problem, the only quantum term of Eq. (6) comes from the third derivative of the quartic term where Eq. (7) gives that the quantum term goes as $\zeta = \hbar^2 \chi^2$; for any other form of the potential, we expect different corrections and hence different scaling as below.

We now use this in an expansion technique for entropy dynamics that may be applied in general. In the Duffing problem, even though $\dot{S}_2$ is not a simple function of ζ, a scaling relationship still obtains in the two parameters $\hbar, D$ as follows. To zeroth order, the classical and quantal phase-space distributions are the same, $\rho_{W0} \approx \rho_c$, and $\chi_{q0}^2 = \chi_c^2$, where the entropy production rate $\dot{S}_{2q0} = -2D\chi_{q0}^2$ and the numerical subscripts on $\chi_q, \rho_W, \dot{S}_{2q}$ indicates the order of the approximation. We now use the results from Eqs. (6) and (7)

that the quantum-classical distance for this system behaves as $\hbar^2 \chi^2$. To first order we insert the zeroth order solution in this to write

$$\rho_{W1} \approx \rho_{W0} + a\hbar^2 \chi^2 \rho_{W0} = \rho_c + a\hbar^2 \chi^2 \rho_c, \quad (8)$$

where a is constant for the metastable state, but time-dependent in general. We substitute this in Eq. (3) to get that $\chi_{q1}^2 \approx \chi_c^2 + a\hbar^2 \chi_c^4$. Corrections from the denominator of Eq. (3) are of higher order, and also tend to cancel the higher order corrections from the numerator. We insert this first order quantally corrected form for the dynamical term into Eq. (4) to get that to first order in $\hbar^2$, χ^2 obeys

$$\frac{d\chi^2}{dt} \approx 2\Lambda(\chi^2 + a\hbar^2 \chi^4) - 4D\chi^4 \quad (9)$$

and in parallel to Eq. (5) we get that

$$\chi^{2*} = \frac{\Lambda}{2D\left(1 - \frac{a\hbar^2}{4D}\right)} \quad (10)$$

leading finally to $\dot{S}_{2q1} = -2D\chi_{q1}^2 = -\Lambda\left(1 + \frac{a\hbar^2}{4D}\right)$ that is, the quantum correction scales as $\hbar^2/D$. This expansion around the metastable state can occur only when the growth of structure is balanced by noise, only when χ^2 is large enough that the diffusion term becomes relevant. Since a is in general time-dependent, at each value of ζ_0 we expect a different entropy dynamics, as in fact we see. In summary, this expansion for the entropy dynamics around the metastable state yields a $\hbar^2/D$ dependence for entropy, although the time-dependence itself is not easy to extract.

This expansion must fail for arbitrarily large ζ_0, in the quantum regime. Here an alternate approach applies: the Poisson bracket term is neglected and the dynamics are given approximately by the competition between the L_q and T terms alone. To compare them, consider L_q: For the Duffing system, there is a third-derivative of ρ_W multiplied by x (resulting in this acting like a second derivative overall), compared to the second derivative from the diffusion term [18]. This means that the terms have essentially the same scale, with quantum dynamics continuing to add structure and the noise smoothing it out. The entropy-production then depends only on the ratio of the parameters multiplying these terms which is again $\hbar^2/D \equiv \zeta_0$. This last parameter regime is consistent with recent results [7,17]. Finally, consider some details of the time dependence: The rate of purity decay decreases with ζ_0. Physically, the time-asymptotic dynamics are dominated by essentially classical diffusive behavior, with a common final state (the natural invariant measure) for all ρ_W. Since $\text{Tr}\{\rho_W^2(0)\} \propto \hbar^{-1}$ (see above), the time-asymptotic value of $\text{Tr}\{\rho_W^2(t)\}/\text{Tr}\{\rho_W^2(0)\} \propto \hbar^{-1}$. With the different rates of purity decay, the system approaches the time-asymptotic state later as ζ_0 increases. Further, within each ζ_0, the different values of $\hbar$ separate out from the scaling curve as the final diffusive regime kicks in, as seen in Fig. 2.

The values of ζ_0 where these regimes change is in general determined by the parameters of the potential, i.e., by the quantity labeled as a in Eq. (8) above. Given the continuous

behavior as a function of ζ_0 the actual transition is subjective. In Fig. 2 we label what corresponds to rapidly decohering and hence essentially classical behavior as (I), the relatively slowly decohering and hence deep quantum behavior as (III) and in-between semiclassical behavior as (II) in the three sets of curves with ($\zeta_0 = 2, 100, 40$), respectively. That is, for this potential, empirically $\zeta_0 = \zeta_c \approx 10$ sets the approximate upper limit of the rapidly decohering regime (I), and by extension the quantum regime (III) kicks in at $\zeta_0 = \zeta_q \approx \zeta_c^2 \approx 100$. We note the same scaling also holds (results not shown) for other diagnostics as well as for very different parameters for the Duffing oscillator, $A = 10$, $\omega = 6.07$, a regime of significantly increased chaos [6].

In conclusion, our results strengthen the argument that it is valuable to study the behavior of nonlinear open quantum systems through the scaling behavior of appropriate diagnostics, as recently suggested [9]. In particular, this is used to study the nonequilibrium statistical mechanics of an open quantum system with a classically chaotic counterpart over a wide parameter range in $\hbar, D$. We show that the entropy dynamics of this system can be dramatically different from the broadly accepted Lyapunov exponent dependence which is only valid in the classical limit (and is itself arguably suspect [11]). We show a $\hbar^2/D$ scaling in the time-dependent entropy dynamics, although the particular form of the scaling is expected to depend on the form of the nonlinearity in general.

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