Lyapunov Exponents, Entropy Production, and Decoherence

Arjendu K. Pattanayak

Department of Physics, Rice University, Houston, Texas 77251-1892
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We establish that the entropy production rate of a classically chaotic Hamiltonian system coupled to the environment settles, after a transient, to a metastable value given by the sum of positive generalized Lyapunov exponents. A metastable steady state is generated in this process. This behavior also occurs in quantum systems close to the classical limit, where it leads to the restoration of quantum-classical correspondence in chaotic systems coupled to the environment.

The Lyapunov exponents of a chaotic classical Hamiltonian system characterize the rate of exponential divergence of neighboring phase-space trajectories thus defining the microscopic time scales. The question [1] of their role in the macroscopic behavior of the system is hence at the foundation of statistical mechanics. It is also of deep interest to understand how the Lyapunov exponents govern the behavior of the quantum counterparts of these chaotic systems [2]. For instance, it is predicted [3] that quantum effects comparable to the classical behavior should be measurable on a time scale $t_B \approx \frac{1}{\lambda} \ln(\frac{1}{\hbar})$. Here $\hbar$ is Planck's constant scaled by a characteristic action for the system and λ is the largest Lyapunov exponent of the system. This "break time" can be ≈ 20 yr for astronomical systems [4] and is clearly incompatible with observations. It is argued [4] that this problem may be resolved by considering the decoherence resulting from including environmental effects on the system evolution. Since this can be understood as a dynamical coarse graining, and statistical properties of the system are typically obtained through a static coarse graining, a diagnostic of common primary interest for both issues is the behavior of the coarse-grained entropy of the system. The Gibbs entropy $S_G = \text{Tr}[\rho \ln \rho]$ and the linear or Renyi entropy $S_2 = \ln(\text{Tr}[\rho^2])$ are both useful [5] in this regard. Here ρ is the classical phase-space probability distribution $\rho^C(x)$ or the quantum quasiprobability Wigner distribution $\rho^W(x)$ as appropriate and Tr denotes the integration over all phase-space variables $x = (q, p)$. These entropies measure the information in the probability distribution and remain constant for Hamiltonian evolution without coarse graining. A change in the coarse-grained entropy corresponds to information being lost at the finest scales. Since in a chaotic system ρ acquires structure at small scales exponentially rapidly [2], $\dot{S}_2$ typically grows exponentially rapidly in magnitude initially for such classical systems, as also for their quantum analogs close to the classical limit [7]. Numerical studies with static coarse graining [8] and the analysis of the behavior of a Gaussian wave packet in the upside-down harmonic oscillator suggest that for weakly coupled systems $\dot{S}_G$ settles to a metastable "constant" after this transient. This metastable value is

conjectured [4] to be the sum $\sum_i \lambda_i^+$ over the positive Lyapunov exponents of the classical system, independent of the details of the original distribution. This conjecture has not yet been verified. Preliminary analyses [9] indicate that systems may become metastable although the quantitative conjecture does not hold in general. In this paper, we consider a variation of this conjecture and are able to analytically establish it for the *general* case of an arbitrary distribution evolving in a chaotic system. We do so by considering the dynamics of the quantity $\chi(t)$ which measures the degree of structure in a phase-space distribution, and is directly proportional to the entropy production rate. We demonstrate that under reasonable approximations the entropy production rate $\dot{S}_2$ indeed settles after an exponential transient to $\dot{S}_2 \approx -\sum_i \Lambda_{2,i}^+$. The $\Lambda_{2,i}$, as defined below, are generalized Lyapunov exponents that depend upon the initial distribution in general. We further show that this is a robust result: Although for sufficiently weakly coupled systems $\dot{S}_2$ *increases* in magnitude to a constant, for a stronger coupling the magnitude of $\dot{S}_2$ starts high and *decreases* to the same constant. The metastable rate is hence independent of the environmental strength. We also generalize the idea that for such systems ρ can evolve to a metastable state [4,10] and show that for such states the quantum corrections for classically chaotic systems remain small for all times, indeed resolving the issue of the anomalously short break time. We thus obtain a condition for the restoration of correspondence through decoherence. Finally, we present numerical results verifying these analytic results for the particular case of the quantum cat map and its classical limit, a uniformly hyperbolic K-system satisfying the assumptions in our arguments [11].

The evolution of ρ^W under the potential $V(q)$ and coupled to an external environment [4,12] is

$$\frac{\partial \rho^W}{\partial t} = \{H, \rho^W\} + \sum_{n \geq 1} \frac{\hbar^{2n}(-1)^n}{2^{2n}(2n+1)!} \frac{\partial^{2n+1} V(q)}{\partial q^{2n+1}}$$
$$\times \frac{\partial^{2n+1} \rho^W}{\partial p^{2n+1}} + D\nabla^2 \rho^W. \tag{1}$$

The first term on the right is the Poisson bracket, generating the classical evolution for ρ^W; the terms in $\hbar$ add

the quantal evolution. The environmental effects are contained in the ∇^2 term; for simplicity we have assumed coupling to all the phase-space variables, although the results can be easily generalized. The parameter D depends strongly upon the form of the coupling and the spectrum of the environment [12]. The entropy production rate is then $\dot{S}_2 = 2D\frac{\text{Tr}[\rho^W \nabla^2 \rho^W]}{\text{Tr}[(\rho^W)^2]} = -2D\frac{\text{Tr}[|\nabla \rho^W|^2]}{\text{Tr}[(\rho^W)^2]} \equiv -2D\chi^2$ where the second equality results from an integration by parts. The global quantity $\chi^2(t)$ corresponds to the mean-square radius of the Fourier expansion of ρ; it hence measures the structure in the distribution [2] and also governs the entropy production rate. To understand the behavior of S_2 first consider the classical Hamiltonian evolution, that is, only the Poisson bracket terms in Eq. (1). In this case, the point dynamics satisfy $\dot{x} = f(x)$ with the accompanying induced flow $x_t = \Phi^t x_0$ and [2] the phase-space gradient along a trajectory is governed by $\nabla\rho(x_t) = -\mathcal{M}(t, x_0)\nabla\rho(x_0)$, where the fundamental matrix $\mathcal{M}$ is given by [1] the time-ordered series $\mathcal{M}(t, x_0) = \mathcal{T} \exp \int_0^t \frac{\partial f(\Phi^\tau x_0)}{\partial x} d\tau$. This defines a real symmetric matrix $\mathcal{M}^T \cdot \mathcal{M}$ (the transpose denoted by $\mathcal{M}^T$) which can be diagonalized [1] as $M^T(t, x_0) \cdot M(t, x_0) = \sum_i u_i(t, x_0)\sigma_i(t, x_0)u_i^T(t, x_0)$, whence the u_i constitute a local orthonormal tangent space for the flow. The local Lyapunov exponents are then given by $\lambda_i(x_0) = \lim_{t\to\infty} \frac{1}{2t} \ln \sigma_i(t, x_0)$. We may now define the global averages

$$\Lambda_{2,i}(\rho, t) = \frac{1}{2t} \ln\left[\frac{\text{Tr}[|\nabla_i \rho(x_0)|^2 \sigma_i(t, x_0)]}{\text{Tr}[\nabla_i \rho(x_0)]^2} \right]$$
$$= \frac{1}{2t} \ln\left[\frac{\text{Tr}[|\nabla_i \rho(x_t)|^2]}{\text{Tr}[\nabla_i \rho(x_0)]^2} \right] \quad (2)$$

and their limits $\Lambda_{2,i}(\rho) = \lim_{t\to\infty}\Lambda_{2,i}(\rho, t)$. The last equality in Eq. (2) comes from the orthonormality of the u_i and the dependence of $\nabla\rho(x_t)$ on $\mathcal{M}$. These Λ are ρ dependent versions of the usual generalized Lyapunov exponents of second order [6] which may be recovered by replacing $|\nabla_i \rho(x_0)|^2$ by the natural invariant measure $\rho_0(x)$ of the dynamics. For linear systems $\sigma_i(t, x_0) = \sigma_i(t)$ and the definitions are independent of ρ. For ergodic dynamics $\Lambda_{2,i}(\rho, t) = \Lambda_{2,i}(\rho)$ for all time. However, numerical evidence suggests that this equality is valid within small errors for "typical" initial densities ρ for other Hamiltonian flows as well. We can always write $\Lambda_{2,i}(\rho, t) = \Lambda_{2,i}(\rho) + \xi_i/t$ where ξ fluctuates in general and ξ/t vanishes with increasing t. The analysis so far has been exact; hereafter we make the approximation of neglecting the ξ term. We now decompose the entropy production rate into the contribution from the different stability subspaces as $\dot{S}_2 = -2D\chi^2 = -2D\sum_i \chi_i^2$ where $\chi_i^2 = \text{Tr}[|\nabla_i \rho(x_t)|^2]/\text{Tr}[\rho^2(x_t)] \equiv \langle k_i^2 \rangle_{\rho_k^2}$ is the i component of χ^2. The preceding enables us to write

$$\frac{d\chi_i^2}{dt} \approx 2\chi_i^2 \Lambda_{2,i} \quad (3)$$

or equivalently $\dot{S}_2 \approx -2D\sum_i \chi_i^2(0)e^{2\Lambda_{2,i}t}$ where the ρ dependence of $\Lambda_{2,i}$ is left implicit hereafter. This shows the initial behavior of $\dot{S}_2$; it is dominated by the largest positive generalized exponent $\Lambda_{2,1}^+$, thus recovering an earlier approximate result [7]. After this initial stage, the structure reaches the finest scales and hence the D-dependent diffusion term becomes important. To include the impact of this we first consider purely diffusive behavior such that $\partial_t \rho = D\nabla^2 \rho$. Since the Laplacian is independent of the coordinate system, this may be decomposed into the same subspaces as above as $\partial_t \rho = D\sum_i \nabla_i^2 \rho$ with the solution being a product of the distributions as $\rho = \Pi_i \rho_i(x_i)$. Each direction has the standard solution written in terms of the Fourier components as $\rho_{k_i} = \rho_{k_i} \exp(-Dk_i^2 t)$ whence the individual $\chi_i^2(t) = \langle k_i^2 \rangle_{\rho_k^2} = \sum_k k_i^2 |\rho_k(0)|^2 \exp(-2Dk^2t)/[\sum_k |\rho_k(0)|^2 \exp(-2Dk^2t)]$ have the time dependence

$$\frac{d\chi_i^2}{dt} = -2D[\langle k_i^4 \rangle_{\rho_k^2} - \langle k_i^2 \rangle_{\rho_k^2}^2]$$
$$\approx -4D\langle k_i^2 \rangle_{\rho_k^2}^2 = -4D\chi_i^4. \quad (4)$$

The approximation in Eq. (4) is a mean-field one, valid for the usual Gaussian solution to the diffusion equation, for example. The various χ_i^2 therefore behave as follows: An initial exponential transient entirely kills these quantities in the stable directions (corresponding to the negative Lyapunov exponents) and since this is enhanced by diffusive effects, these directions have a negligible role thereafter. In the unstable directions, however, the initial exponential growth is balanced by the diffusion. If we now explicitly set $d\chi_i^2/dt$ equal to the sum of the chaotic [Eq. (3)] and diffusive [Eq. (4)] terms, we get $\frac{d\chi_i^2}{dt} = 2\Lambda_{2,i}^+\chi_i^2 - 4D\chi_i^4$ for the unstable directions. This has the stationary solution $\chi_i^{2*} = \Lambda_{2,i}^+/2D$ yielding the stationary entropy production rate $\dot{S}_2^* = -2D\chi^{2*} = -2D\sum_i \chi_i^{2*} = -\sum_i \Lambda_{2,i}^+$ with the sum over the positive exponents only, as just argued. Thus, within the approximations as above, we have shown that the entropy production rate for a chaotic system weakly coupled to the environment settles after an initial exponential transient to a metastable value as above, independent of the precise magnitude of the environmental effects [13]. This solution is stable under small pertubations; thus, the exact dynamics arguably leave it unaltered. We now consider possible constraints on this result. First, note that the transition from the exponential to the linear regimes happens at $t_i^* \approx (1/2\Lambda_{2,i}^+)\ln[\Lambda_{2,i}^+/2D\chi_i^2(0)]$ (the shortest scale is approximated by the largest exponent $\Lambda_{2,1}^+ \equiv \lambda$ and the full χ^2 and we shall use those hereafter). Since $t^* = 0$ for $\beta \equiv 2\lambda^{-1}D\chi^2(0) = 1$, for $\beta \gg 1$, the initial behavior of χ_i^2 is not the exponential transient but is given by Eq. (4) instead. For this case, the initial diffusive effects are balanced by the chaos such that an initially large $\dot{S}_2$ decreases to a constant. Second, the difference between the initial entropy $S_2(0)$ and the final entropy $S_2(\infty)$ is

typically finite. Thus, the system may not have "enough initial entropy" to evolve to the constant entropy rate as above. A rough estimate (and numerical results as described below) indicates that we need $S_2(0) - S_2(\infty) > 3$ for the linear saturation behavior to emerge [14]. Finally, in contrast to this behavior for chaotic systems, a similar analysis for nonchaotic systems yields an initial nonexponential decay of S_2 after which the competition from the diffusive term implies a maximum ($\propto D^{-1}$) for $\dot{S}_2$, and a rapid decrease thereafter. As a result of these dynamics, appropriate initial distributions ρ for chaotic systems settle to a metastable state with χ_i^2 as above. This is a remarkable result, generalizing earlier arguments [4,10] for a "steady-state Gaussian width." Further, this enables us to bound the quantum corrections in Eq. (1). Consider the first quantum term in Eq. (1), which scales as $\hbar^2 \chi^3$. In the absence of the D-dependent terms, χ grows exponentially rapidly as $\exp(\lambda t)$, thus leading to a quantum-classical break time $t_b \approx \frac{1}{\lambda} \ln(\frac{1}{\hbar})$ after which the quantum "correction" is comparable to the classical evolution and a classical description of the dynamics is invalid. This logarithmic dependence of t_b on $\hbar$ is extremely weak and is a point of debate in the analysis of quantum chaotic systems [4]. However, environmental effects saturate χ and hence the first quantum term at $\zeta \approx \hbar^2 (\lambda/2D)^{3/2}$ such that this indeed is a correction of $\mathcal{O}(\hbar^2)$ to the classical evolution and there is no break time. The condition [15] for restoration of quantum-classical correspondence for chaotic systems may be summarized as $\zeta \ll 1$ (note that the other quantum terms are higher order in ζ). Physically, quantum effects are important at the smallest scales $\approx \hbar$ of phase space. Classically chaotic evolution increases the support of a distribution at the finest scales exponentially rapidly, thus enhancing quantum effects. However, noise or coarse graining washes out the details of the fine-scale structure, thus restoring quantum-classical correspondence [16]. For systems where the above inequality is violated, however, a classical or semiclassical analysis breaks down and we must use the exact quantum evolution.

We have numerically verified the theory using the equivalent of Eq. (1) for the classical and quantum cat map [11]. As this system is linear and ergodic, the approximations above hold exactly. Some of the data obtained are shown in Figs. 1–3. First, with a scaled Planck's constant $2\pi\hbar = 10^{-5}$, we expect [11] essentially classical behavior, even with no added noise. This is indeed verified as in Fig. 1 where the classical data for the same initial conditions and D exactly overlie the quantum results. For an initial sharply localized Gaussian state, corresponding to high initial entropy, when D is small we see initial exponential entropy production [7]; this saturates to linear behavior with the predicted slope. The initial exponential behavior is swamped as D is increased, as argued previously. For a second initial state which is spread out and has lower initial entropy, we see similar stable behavior—although $\dot{S}_2$ now satu-
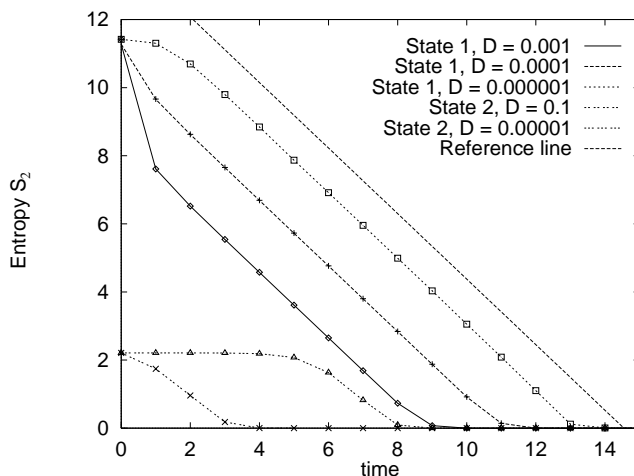

FIG. 1.   Time dependence of the entropy $S_2(t)$ for the chaotic cat map for varying levels of coupling to the environment, as measured by D. Classical and quantal ($2\pi\hbar = 10^{-5}$) numerics were run for identical initial conditions and noise strengths D. The classical results are shown as points overlaid on the lines for the corresponding quantal data. There are two different initial conditions, one with high initial entropy $S_2(0)$ and the other with lower $S_2(0)$. A reference line with slope equal to $\Lambda_2 = 0.9624$ is also shown.

rates earlier, as discussed above—confirming that this metastability is essentially independent of initial conditions and of D for near-classical systems. Figure 2 shows the quantum-to-classical transition by comparing various runs for a single sharply localized initial condition at $2\pi\hbar = 10^{-3}$ with their classical equivalents. We see that for very small D (hence large ζ) there is significant quantal deviation from the classical behavior. However, as D is increased (and ζ correspondingly decreases below 1),
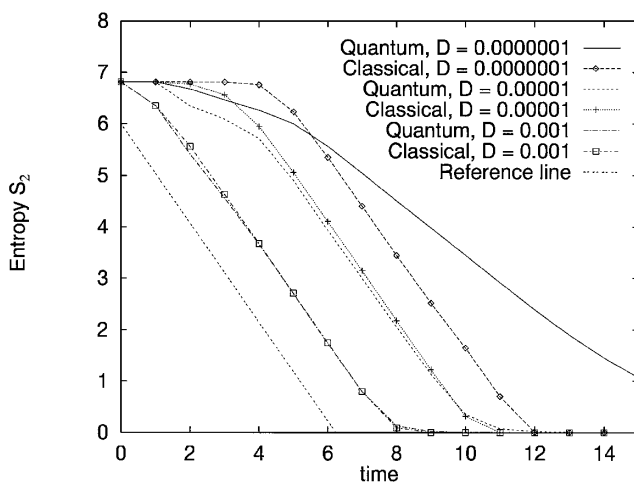

FIG. 2.   Quantal and classical results are shown with $2\pi\hbar = 10^{-3}$, a single initial condition and varying D. As D is increased, the quantal behavior approaches that of the classical system. As in Fig. 1, a reference line with slope equal to $\Lambda_2 = 0.9624$ is also shown.
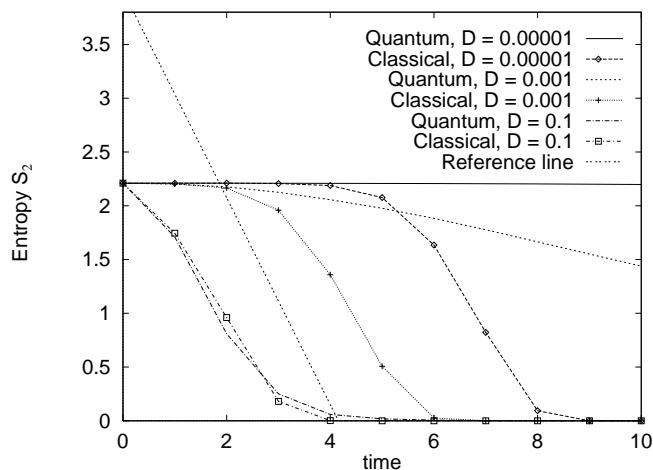
FIG. 3.   As in Fig. 2, but with $2\pi\hbar = 10^{-1}$. The quantal system is almost unaffected by small D. The quantal behavior tends to the classical with increasing D; however, it is then dominated by noise and the slope is always less than that of the reference line shown with slope of $\Lambda_2 = 0.9624$.

the quantal $\dot{S}_2$ approaches the classical linear saturation behavior as above. A more spread-out initial distribution has the same qualitative behavior (not shown) except that it saturates early as expected. We note that the distributions for both Figs. 1 and 2 are *not* Gaussian during the metastable stage of the dynamics. Figure 3 shows results for $2\pi\hbar = 0.1$. Here the uncertainty principle constrains the initial ρ to occupy a substantial portion of the available phase space. We see again that for $\zeta \gg 1$, the quantum behavior is substantially different from the classical and there is almost no sensitivity to the environment (low entropy production). As D increases, quantum-classical correspondence is indeed restored, although D is now so large the dynamics are essentially that of the noise alone and $\dot{S}_2$ saturates at less than Λ_2. The abruptness of the tail in all our computations is most probably a numerical artifact due to the extremely small numbers being computed at that time; a detailed understanding of this tail is still absent. These results show that the entropy production rate for an arbitrary distribution in classically chaotic system saturates, after an exponentially rapid transient, to the sum of the positive generalized Lyapunov exponents of the system; further, the distribution settles to a metastable state. This is a clear signature of the underlying chaos, stable against perturbation. This behavior is echoed by quantum systems close to the classical limit, and the satu-

ration is the precursor for quantum-classical correspondence in chaotic systems coupled to the environment.

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