Complexity and nonseparability of classical Liouvillian dynamics

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We propose a simple complexity indicator of classical Liouvillian dynamics, namely the separability entropy, which determines the logarithm of an effective number of terms in a Schmidt decomposition of phase space density with respect to an arbitrary fixed product basis. We show that linear growth of separability entropy provides a stricter criterion of complexity than Kolmogorov-Sinai entropy, namely it requires that the dynamics be exponentially unstable, nonlinear, and non-Markovian.

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I. INTRODUCTION

How can one characterize the algorithmic complexity of Liouville evolution $\mathrm{d}\rho^t/\mathrm{d}t = \{\rho^t, H\}_{\text{Poisson bracket}}$ of conservative classical dynamics with Hamiltonian H? Is Kolmogorov-Chaitin complexity of individual orbits related to the complexity of field solutions $\rho^t(z)$ (z denoting a collection of $2d$ phase space coordinates) of the Liouville equation? The answer is "no," as shown by a paradigmatic example of chaotic dynamics, the stretching and folding baker's map, which is equivalent to the Bernoulli shift on an infinite binary symbol sequence (coin tossing), so its orbit dynamics is algorithmically complex but its Liouville evolution is exactly solvable [1]. More generally, one can identify two extreme cases of exact solvability in conservative (closed and noiseless) classical dynamics, namely (i) orbitwise exact solvability, which is associated with a Liouville *integrability* and the existence of a complete set of constants of motion, and (ii) fieldwise exact solvability, which is associated with the existence of a finite Markov partition and symbolic dynamics [2,3].

The fundamental question that we address in this paper is whether the notion of complexity qualitatively changes when we focus our attention from individual orbits to time-dependent statistical ensembles. The latter is more common and meaningful in statistical mechanics. We propose to apply a concept of a Schmidt rank and entanglement entropy—common in quantum-information theory [4]—to a joint probability distribution of several classical (dynamical) variables in order to describe the growth rate of complexity of the description of classical field solutions of the Liouville equation. In this way, a new and conceptually very simple measure of complexity is defined, *the separability complexity*, which exactly vanishes in both cases (i,ii) of exact solvability and thus hopefully detects genuinely hard cases of classical deterministic dynamics, even in the statistical sense. The utility of the new measure is demonstrated and compared to the characteristics of the transport and diffusion in Fourier space (being common measures of Hamiltonian turbulence) for several nontrivial examples of chaotic and regular two-dimensional (2D) and four-dimensional (4D) classical dynamical maps. One should note that introducing either *classical noise* or *quantum effects* introduces a natural cutoff scale to a phase space resolution and thus qualitatively reduces such a notion of complexity. Quantum or noisy classical dynamics can become genuinely complex only in the (thermodynamic) limit of increasingly many degrees of freedom.

II. SEPARABILITY ENTROPY AND COMPLEXITY INDICATORS

To make our discussion simple but general, we shall consider discrete dynamical systems, say stroboscopic or Poincaré maps of Hamiltonian dynamics, given in terms of a Lebesgue-measure preserving invertible map $z_{t+1} = \boldsymbol{\phi}(z_t)$ over a compact phase space $\mathcal{M} \subset \mathbb{R}^{2d}$. The map induces a *unitary* Perron-Frobenius operator over the Hilbert space $L^2(\mathcal{M})$ of phase space densities, $(\hat{U}\rho)(z) \equiv \rho[\boldsymbol{\phi}^{-1}(z)]$. For simplicity, we shall identify the phase space with a $2d$-dimensional torus $\mathcal{M} = \mathbb{T}^{2d}$ (while more general cases can be treated with obvious modifications) and consider an arbitrary phase space decomposition $\mathcal{M} = \mathbb{T}^d \oplus \mathbb{T}^d \ni \boldsymbol{z} \equiv (\boldsymbol{x},\boldsymbol{y})$ into two sets of d coordinates, which could, for example, describe two disjoint subsets of degrees of freedom, or $\boldsymbol{x}$ could be positions and $\boldsymbol{y}$ momenta, etc. The phase space decomposition induces factorization of the Hilbert space of densities $L^2(\mathcal{M}) = L^2(\mathbb{T}^d) \otimes L^2(\mathbb{T}^d)$. Let us write the time-evolved Liouville density as $\rho^t(\boldsymbol{x},\boldsymbol{y}) = (\hat{U}^t\rho^0)(\boldsymbol{x},\boldsymbol{y})$ and normalize it in an L^2 sense as $\int \mathrm{d}^{2d} z |\rho^t(z)|^2 = 1$. Then we write the Schmidt (or *singular value*) decomposition of the density,

$$\rho^t(\boldsymbol{x},\boldsymbol{y}) = \sum_n v_n^t(\boldsymbol{x}) \mu_n^t w_n^t(\boldsymbol{y}), \tag{1}$$

in terms of two sets of *orthonormalized* functions $\{v_n^t\}$, $\{w_n^t\}$, $n = 1,2\ldots$ and a set of Schmidt coefficients $\{\mu_1^t \geqslant \mu_2^t \geqslant \cdots \geqslant 0\}$ satisfying $\sum_n |\mu_n^t|^2 = 1$. In practice, we can treat $\rho^t(\boldsymbol{x},\boldsymbol{y})$ as a matrix of row $\boldsymbol{x}$ and column $\boldsymbol{y}$ and consider sufficiently fine discretization of continuous variables $\boldsymbol{x},\boldsymbol{y} \in \mathbb{T}^d$ so that the results do not depend on it. Let us define a *separability entropy* (s-entropy) as a logarithm of an effective number of terms in decomposition (1),

$$h[\rho^t] = -\sum_n |\mu_n^t|^2 \ln |\mu_n^t|^2, \tag{2}$$

which gives a quantitative measure of separability of phase space density with respect to a given phase space decomposition [5]. Alternatively, $h[\rho^t]$ can be computed as von Neuman entropy $h[\rho^t] = -\mathrm{tr}[R^t \ln R^t]$, where R^t are trace-class, positive, self-adjoint operators on $L^2(\mathbb{T}^d)$ with integral kernels $R^t(\boldsymbol{x},\boldsymbol{x}') = \int \mathrm{d}^d \boldsymbol{y} \rho^t(\boldsymbol{x},\boldsymbol{y})\rho^t(\boldsymbol{x}',\boldsymbol{y})$. Note that s-entropy $h[\rho^t]$

does *not* depend on the coordinate system we use for each phase space factor space, since decomposition (1) is invariant under invertible measure-preserving transformations of the form $(\boldsymbol{x},\boldsymbol{y}) \to (\boldsymbol{\chi}(\boldsymbol{x}),\boldsymbol{\eta}(\boldsymbol{y}))$, namely it only depends on phase space decomposition and dynamics $\boldsymbol{\phi}$. A nontrivial phase space decomposition can be generated from a canonical one in terms of some phase space diffeomorphism $\boldsymbol{\pi}:\mathcal{M}\to\mathcal{M}$, namely $\boldsymbol{z}=\boldsymbol{\pi}(\boldsymbol{x},\boldsymbol{y})$, and the corresponding s-entropy is computed as $h[\rho^t\circ\boldsymbol{\pi}]$. Now, let us assume that for sufficiently complex dynamics, s-entropy can grow proportionally with time, and define its asymptotic growth rate as *s-complexity*,

$$C_{\rm s}[\boldsymbol{\phi}] = \inf_{\pi}\sup_{\rho^0}\lim_{t\to\infty}\frac{1}{t}h[\rho^0\circ\boldsymbol{\phi}^{-t}\circ\boldsymbol{\pi}], \tag{3}$$

taking first a supremum over initial densities ρ^0 and later an infimum over the phase space decompositions $\boldsymbol{\pi}$ [6]. Clearly, *any* complete and accurate (numerical) representation of phase space density ρ^t needs at least $O(\exp(h[\rho^t]))$ terms of the form (1), so $O(\exp(C_{\rm s}t))$ estimates [7] the necessary amount of classical computing resources needed to simulate Liouville dynamics up to time t, but is it *sufficient*?

As an alternative measure of algorithmic complexity of Liouville dynamics, we define the *Fourier entropy* (f-entropy) as the logarithm of an effective number of Fourier harmonics $\tilde{\rho}^t(\boldsymbol{k}) \equiv (2\pi)^{-2d}\int d^{2d}z e^{i\boldsymbol{k}\cdot\boldsymbol{z}}\rho^t(\boldsymbol{z})$, $\boldsymbol{k}\in\mathbb{Z}^{2d}$, needed to simulate the solution for time t, namely

$$g[\rho^t] = -\sum_{\boldsymbol{k}\in\mathbb{Z}^{2d}}|\tilde{\rho}^t(\boldsymbol{k})|^2\ln|\tilde{\rho}^t(\boldsymbol{k})|^2, \tag{4}$$

and the corresponding *f-complexity* as

$$C_{\rm f}[\boldsymbol{\phi}] = \sup_{\rho^0}\lim_{t\to\infty}\frac{1}{t}g[\rho^0\circ\boldsymbol{\phi}^{-t}]. \tag{5}$$

$O(\exp(C_{\rm f}t))$ gives a *sufficient* amount of classical computing resources needed for accurate simulation of Liouville dynamics up to time t, but is it *necessary*? Summarizing, we state the following two inequalities:

$$C_{\rm s} \leqslant C_{\rm f} \leqslant 2d\lambda_{\max}, \tag{6}$$

where $\lambda_{\max}$ is the maximal Lyapunov exponent which determines the smallest scale $\sim\exp(-\lambda_{\max}t)$ on which $\rho^t(\boldsymbol{z})$ can vary, in each of $2d$ phase space directions.

For the first inequality (6) to be saturated, it would mean that both s-complexity and f-complexity yield a sufficient and necessary amount of computing resources for Liouvillian simulation. As indicated later in numerical experiments, this may not generally be true. For the second inequality (6) to be saturated, it is required that the one-dimensional unstable manifold along the maximally unstable Lyapunov direction densely covers a finite-measure portion of the $2d$-dimensional phase space, and moreover, that the exploration of the modes of the Fourier space is not sparse, as it is, for example, in the case of linear automorphisms on the torus (*cat maps*). This may typically be the case—as indicated later—at least in low-dimensional maps.

It is interesting to note that for any map with a *finite Markov partition*—and thus admitting exact symbolic dynamics with a finite grammar—we have $C_{\rm s}=0$ since in the Markov coordinates the separability [or the number of terms in (1)] is preserved. For linear toral (cat) maps, we even have $C_{\rm f}=0$ since the number of Fourier harmonics is preserved in time even though their magnitude may be growing. Positive s-compexity, $C_{\rm s}>0$, thus represents a very strong condition implying practical unsolvability of Liouville dynamics due to chaotic motion *and* nonexistence of a finite Markov partition.

III. NUMERICAL EXAMPLES

Let us now illustrate our concepts by discussing a set of numerical experiments. Firstly, we consider four different examples of 2D ($d=1$) symplectic toral maps, $(x',y')=\boldsymbol{\phi}(x,y)$: (i) *perturbed cat map* (PC) (as in [8]) $y'=y+x-\alpha\sin x, x'=x+y'$ with $\alpha=0.5$ as an example of a nonlinear, non-Markovian but uniformly hyperbolic Anosov system; (ii) *nonsymmetric standard map* (SM) $y'=y+\alpha\sin x+\beta\cos(2x), x'=x+y'$ with $\alpha=2,\beta=2$ as an example of a strongly chaotic but nonuniformly hyperbolic system with small islands of regular motion of negligible area; (iii) *integrable (Suris) map* [9] (IM) $x'=2x+4\arg(1+\alpha e^{-ix})-y, y'=x$ with $\alpha=0.5$ as an example of a nontrivially integrable map with a separatrix; and (iv) *triangle map* [10] (TM) $y'=y+\alpha\,\mathrm{sgn}(x-\pi)+\beta, x'=x+y'$ with $\alpha=\pi(\sqrt{5}-1)/2, \beta=\pi e^{-1}$ as an example of a dynamically mixing system without exponential sensitivity (all assignments understood mod 2π). In Fig. 1, we show time-evolving phase space densities ρ^{-t} for all four maps at $t=3,5,7$, all starting from the same simple initial density $\rho^0(x,y)=(2+\cos x+\cos y)(2\pi\sqrt{5})$. Note that the three maps PC, SM, and TM exhibit dynamical mixing behavior, although for TM the mixing mechanism is qualitatively different [11]. Only the orbits of the first two maps (PC and SM) have positive Kolmogorov complexity, with estimated Lyapunov exponents (being equal to Kolmogorov-Sinai entropies) $\lambda_{\max}^{\rm PC}=0.9496$, $\lambda_{\max}^{\rm SM}=0.8206$, and only PC exhibits exponential decay of correlations, $\int d^2z\rho^0(z)\rho^t(z)-1\sim\exp(-\xi t)$, with $\xi^{\rm PC}=1.17$, while for SM and TM correlations decay as power laws.

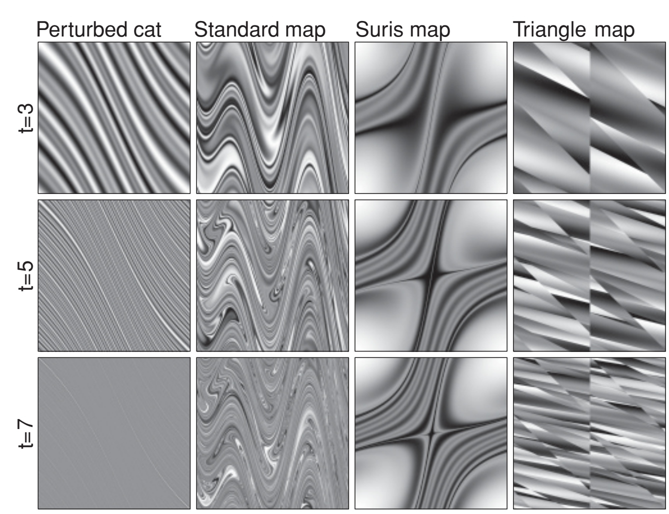

FIG. 1. Snapshots at $t=3,5,7$ (top-down) of Liouville dynamics starting from initial density $\rho^{t=0}(x,y)=(2+\cos x+\cos y)(2\pi\sqrt{5})$ for the four 2D toral maps (PC, SM, IM, TM, left-right) introduced in the text. The gray scale indicates the probability density $\rho^t(x,y)$ (zero is white, maximal is black).

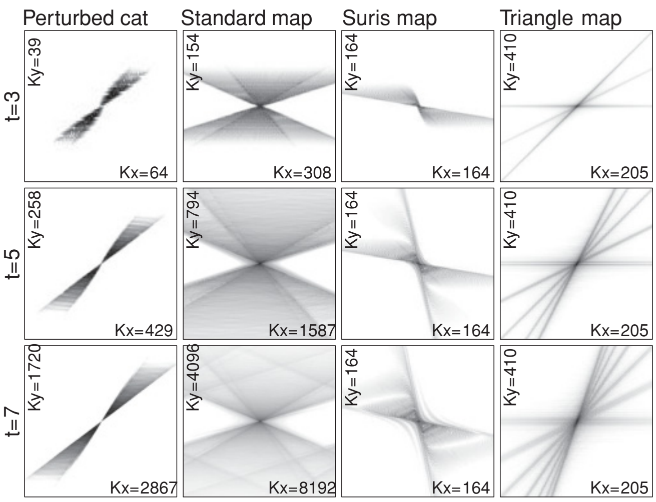

FIG. 2. Snapshots at $t = 3,5,7$ (top-down) of Liouville density in Fourier space $\tilde{\rho}^t(k_x,k_y)$, starting from $\tilde{\rho}^0(k_x,k_y) \propto 4\delta_{k_x,0}\delta_{k_y,0} + \delta_{|k_x|,1}\delta_{k_y,0} + \delta_{k_x,0}\delta_{|k_y|,1}$, for the four different 2D toral dynamics (PC, SM, IM, TM, left-right) introduced in the text. The gray scale indicates probability density (zero is white, maximal is black), while axes labels K_x and K_y indicate the Fourier space range $[-K_x,K_x] \times [-K_y,K_y]$, which is scaled (both in the x and y directions) with the map's Lyapunov exponent $\exp(t\lambda_{\max})$ from the top to bottom panels.

In Fig. 2, we display the corresponding Fourier transformed densities $\tilde{\rho}^{-t}$ to demonstrate the exponential expansion of the distributions of Fourier harmonics in the chaotic cases (PC,SM), resulting in a positive f-complexity. Indeed, as we show in Fig. 3, the f-entropy grows linearly with the upper bound Lyapunov rate (6), namely $C_{\mathrm{f}} = 2\lambda_{\max}$, which

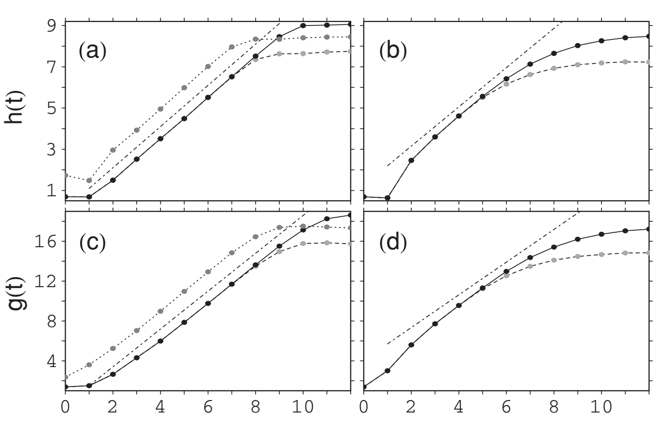

FIG. 3. Separability entropy $h(t) = h[\rho^t]$ (a,b) and Fourier entropy $g(t) = g[\rho_t]$ (c,d) for two cases of chaotic dynamics, PC (a,c) and SM (b,d). Discretization (truncation) with $N = 2^p$ nodes in real (Fourier) space along each (x and y) direction is used, and data for $p = 14$ (black, full curves and symbols), $p = 13$ (dark gray, short dash), and $p = 12$ (light gray, long dash) are shown. For $p = 12,14$ we use the same initial density ρ^0 as in Figs. 1 and 2, while for $p = 13$ (only for PC) a different initial state with Fourier harmonics populated up to $|\boldsymbol{k}| = 4$ is used to demonstrate the same asymptotic growth rates, indicated with dash-dotted lines: $C_{\mathrm{s}} = 1.00$ (a), $C_{\mathrm{s}} = 0.952$ (b), $C_{\mathrm{f}} = 2\lambda_{\max}^{\mathrm{PC}} = 1.90$ (c), $C_{\mathrm{f}} = 2\lambda_{\max}^{\mathrm{SM}} = 1.64$ (d).

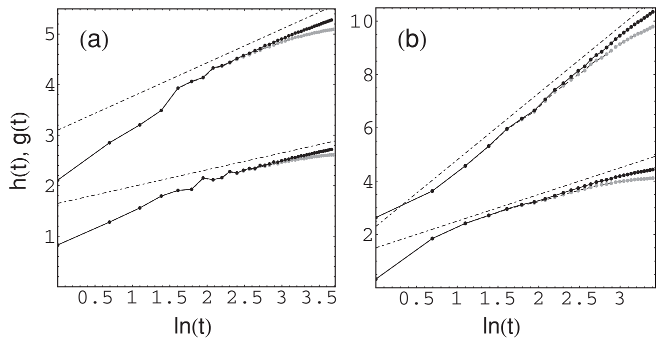

FIG. 4. Separability entropy $h(t) = h[\rho^t]$ (lower curves) and Fourier entropy $g(t) = g[\rho_t]$ (upper curves) for nonchaotic dynamics, integrable IM (a), and nonintegrable TM (b). Data for discretization dimension $N = 2^p$ with $p = 14$ (black curves) and $p = 12$ (gray curves) are shown, where dash-dotted lines suggest asymptotic logarithmic growths $\sim \xi \ln t$, with $\xi = 0.333$ (s-entropy for IM), $\xi = 0.667$ (f-entropy for IM), $\xi = 1.0$ (s-entropy for TM), and $\xi = 2.5$ (f-entropy for TM).

we believe should be a generic behavior for chaotic maps, whereas for s-complexity we find consistently smaller values $C_{\mathrm{s}}^{\mathrm{PC}} = 1.00$, $C_{\mathrm{s}}^{\mathrm{SM}} = 0.952$. Note that completely different behavior is found for linear chaotic maps, or maps with exact symbolic dynamics like the unperturbed cat map or the baker's maps, where we find $C_{\mathrm{s}} = 0$. In nonchaotic maps (IM,TM) we find zero s- or f-compexity, where the temporal growth of s- or f-entropy is likely to be logarithmic (see Fig. 4 and its caption for details).

The numerical results on s-complexity are supplemented by showing the temporal snapshots of the full Schmidt spectrum μ_n^t in Fig. 5. In the chaotic cases (PC, SM) with positive s-complexity, the full spectrum asymptotically scales as $\mu_n^t \propto f[n/(C_{\mathrm{s}}t)]$, and the tail of $f(x)$ decays faster than the power law, while in the regular or nonchaotic cases (IM, TM), μ_n^t converges, as $t \to \infty$, to a universal power-law profile $\mu_n^t \to \mathrm{const}/n$.

Secondly, we consider an example of 4D ($d = 2$) toral automorphism, a simple extension of a perturbed cat map to

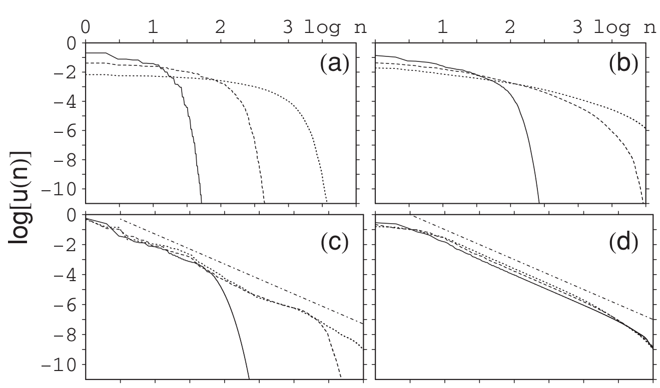

FIG. 5. Singular value (Schmidt) spectra as a function of time for $t = 3$ (full curves), $t = 5$ (long dashed), and $t = 7$ (short dashed), for the dynamics: PC (a), SM (b), IM (c), and TM (d) using discretization dimension $N = 2^{14}$. Base-10 logarithm $\log_{10} u(n)$ of $u(n) = |\mu_n^t|^2$ is plotted against $\log_{10} n$, and in nonchaotic cases (c,d), the dash-dotted line indicates $u(n) \propto 1/n^2$ scaling.

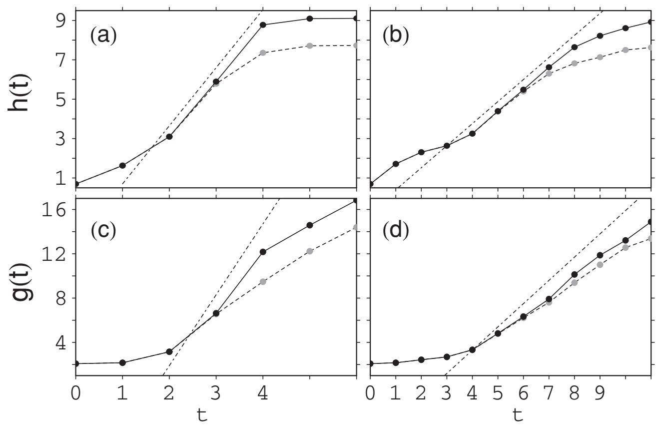

FIG. 6. Separability entropy $h(t) = h[\rho^t]$ and Fourier entropy $g(t) = g[\rho^t]$ for 4D perturbed cat maps: doubly hyperbolic (DH) (a) and loxodromic (Lo) (b). We take discretization and truncation to $N = 2^p$ nodes in each of four phase space directions with $p = 7$ (black, full curves) and $p = 6$ (gray, dashed curves), initial state described in text. The dot-dashed straight lines give the suggested asymptotic rates, $C_s^{\rm DH} = 2.95$ (a), $C_s^{\rm Lo} = 1.12$ (b), $C_f^{\rm DH,Lo} = 4\lambda_{\max}^{\rm DH,Lo}$ (c,d).

$\mathbb{T}^4$, $\boldsymbol{\phi}(z) \equiv (z_1' + \beta_1 \sin z_3', z_2' + \beta_2 \sin z_4', z_3', z_4')$, and $\boldsymbol{z}' \equiv \mathbf{C}\boldsymbol{z}$. As for the linear part, we take exactly the same two cases as in Ref. [12], namely the *doubly hyperbolic* (DH), and *loxodromic* (Lo) cases, with 4×4 matrices

$$\mathbf{C}_{\rm DH} = \begin{pmatrix} 2 & -2 & -1 & 0 \\ -2 & 3 & 1 & 0 \\ -1 & 2 & 2 & 1 \\ 2 & -2 & 0 & 1 \end{pmatrix},$$

$$\mathbf{C}_{\rm Lo} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & -1 & 1 & 1 \\ -1 & -1 & -2 & 0 \end{pmatrix},$$

and we take *nonlinearities* $\beta_1 = 0.2, \beta_2 = 0.3$, resulting in, respectively, maximal Lyapunov exponents $\lambda_{\max}^{\rm DH} = 1.60$ and $\lambda_{\max}^{\rm Lo} = 0.525$. Decomposing $\boldsymbol{x} = (z_1, z_2)$, $\boldsymbol{y} = (z_3, z_4)$, we show in Fig. 6 numerical simulation of s- and f-entropy, starting from the initial state with random lowest Fourier harmonics, i.e., $\tilde{\rho}_{\boldsymbol{k}}^0$ being independent random complex Gaussian variables for $\boldsymbol{k} \cdot \boldsymbol{k} \leqslant 1$ and $\tilde{\rho}_{\boldsymbol{k}}^0 = 0$ otherwise. Again, we obtain, consistently with the 2D case, that the f-entropy grows at a rate that is close to $4\lambda_{\max}$, saturating the second bound in (6), and that the s-complexity is systematically substantially smaller but positive, namely $C_s^{\rm DH} = 2.95$, $C_s^{\rm Lo} = 1.12$.

It should be noted that our numerical experiments provide only partial support for the meaningfulness of the definitions and conjectures stated in Sec. II, although the results seem very suggestive. For example, the supremum over initial density ρ^0 has been tested by increasing the Fourier support of ρ^0, which typically did not result in an appreciable difference in the asymptotic growth rate of $h[\rho^t]$. On the other hand, we have not yet been able to address systematically the infimum over the phase space partitions π in the definition (3). However, several trials of varying π indicated that the numerical result—the value of C_s—may indeed be insensitive to composing with (smooth) π, whereas it seems very plausible that for nonsmooth π the asymptotic growth rate of $h[\rho^0 \circ \boldsymbol{\phi}^{-t} \circ \boldsymbol{\pi}]$ cannot lower. Furthermore, it would be a future challenge to come up with examples of s-complex Liouville dynamics where the positivity $C_s > 0$ could be rigorously proven.

IV. CONCLUSION

We have proposed a simple quantitative measure of complexity of classical nondissipative Liouvillian dynamics. The so-called separability entropy (whose asymptotic growth rate defines what we call s-complexity) is inspired by the entanglement entropy [4] of quantum states, adapted to classical joint probability distributions of several, or many, variables. Note that a similar complexity measure in the *quantum Liouville space* (or operator space) has been used as an indicator of quantum dynamical complexity and *quantum chaos* [13]. It has been argued here that the separability entropy measures the minimal amount of computation resources needed to simulate the classical Liouvillian evolution. Based on simple numerical examples of discrete time dynamical systems on 2D and 4D compact phase space, we have demonstrated that s-complexity is nontrivial and typically smaller than the exponential growth rate of the number of Fourier harmonics (f-complexity). For example, for Hamiltonian dynamics with many degrees of freedom, one might encounter interesting situations with strong Hamiltonian turbulence (large f-complexity), which may be efficiently simulable by a *classical* version of time-dependent density-matrix renormalization group (in the manner of [14]) if s-complexity is small. Our concept is fundamentally different from other popular complexity measures in chaos theory, such as the Kolmogorov-Sinai entropy, that characterize the complexity of individual trajectories and often fail to provide any meaningful complexity information about the time-dependent Liouvillian density.

Our concepts have interesting quantum extensions. We note that f-complexity has already been used to characterize the complexity of quantum time evolution in terms of a Wigner function [15]. We suggest that s-complexity could have a similar quantum phase space extension, but it would provide a sharper discriminant between quantum chaotic and quantum regular motions.

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