Evolution of Liouville density of a chaotic system

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Abstract

An area-preserving map of the unit sphere, consisting of alternating twists and turns, is mostly chaotic. A Liouville density on that sphere is specified by means of its expansion into spherical harmonics. That expansion initially necessitates only a finite number of basis functions. As the dynamical mapping proceeds, it is found that the number of non-negligible coefficients increases exponentially with the number of steps. This is to be contrasted with the behavior of a Schrödinger wave function which requires, for the analogous quantum system, a basis of fixed size.

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I. INTRODUCTION

Chaos is commonly associated with nonlinear dynamics, and the elusiveness of quantum chaos is sometimes attributed to the fact that Schrödinger’s equation is linear. However, the different behaviors of classical and quantum systems cannot be explained so simply. Any classical Hamiltonian motion can be described by means of a (possibly singular) Liouville density, and the evolution of the latter obeys a linear equation, which can be written as

$$i \frac{\partial f}{\partial t} = Lf. \quad (1)$$

Here, $f$ is a function of the $q^n$ and $p_n$, which are independent variables parametrizing phase space, and $L$ is the Liouville operator, or Liouvillian,

$$L = \sum_n \left( \frac{\partial H}{\partial p_n} \right) \left( -i \frac{\partial}{\partial q^n} \right) - \left( \frac{\partial H}{\partial q^n} \right) \left( -i \frac{\partial}{\partial p_n} \right). \quad (2)$$

This operator is formally “Hermitian” (over a suitable domain of Liouville functions $f$) so that the time evolution of $f$ is a unitary mapping of phase space. Namely, if there is another Liouville function, $g$, which also satisfies Eq. (2), the scalar product $\int f^*g \prod dq^n dp_n$ is invariant in time. This is Koopman’s theorem [1].

The essential difference between the Liouville equation and the Schrödinger equation is that, in the generic non-integrable case, the spectrum of the Liouvillian is continuous [2]. This gives rise to fundamental differences between the evolution of Liouville densities and that of quantum wave functions for bounded systems that have discrete spectra in quantum theory. In particular, any quantum state can always be represented, with arbitrary accuracy, by a finite number of energy eigenstates. The time evolution of a bounded quantum system therefore is multiply periodic, and will sooner or later have recurrences [3]. On the other hand, the Liouville equation involves a continuous spectrum, and the evolution of a Liouville density cannot be represented by a finite number of terms.
Thanks to this property, a Liouville density is able to become more and more convoluted with the passage of time, and it may form intricate shapes with exceedingly thin and long protuberances, something that a quantum wave function cannot do [4].

The purpose of this work is to apply to the Liouville equation some of the mathematical techniques that are standard in quantum mechanics. The Liouville density \( f \) is expanded into a complete set of orthonormal functions,

\[
    f(q, p) = \sum_n c_n u_n(q, p).
\]  

(3)

(Note that these \( u_n \) are not the eigenfunctions of the Liouvillian—the latter are not normalizable since its spectrum is continuous.) The Liouville equation (1) then becomes

\[
i \frac{dc_n}{dt} = \sum_n L_{mn} c_n,
\]  

(4)

where \( L_{mn} \) is a Hermitian matrix of infinite order. It follows that \( \sum |c_n|^2 \) is constant in time. However, even if we start with a small number of nonvanishing \( c_n \), it turns out, as will be seen below, that as time passes \( f \) spreads over more and more \( u_n \). A convenient quantitative measure of this spread is the entropy-like expression

\[
S = -\sum_n |c_n|^2 \log |c_n|^2.
\]  

(5)

This \( S \) is analogous to the “entropy” used in the study of quantum chaos [5]. The intuitive meaning of \( S \) is that \( e^S \) is a rough indication of the number of basis vectors that are appreciably involved in the expansion of \( f \) in Eq. (3). An appropriate name for \( S \) could be “dimensional entropy” (or \( D \)-entropy).

Since chaotic systems are characterized by the exponential divergence of neighboring trajectories, we expect that the number of basis functions needed for representing \( f \) (with a given level of accuracy) should also increase exponentially with time. In other words, we expect \( S \) to increase linearly with time for chaotic systems (in the asymptotic limit of
large $t$). On the other hand, for regular systems, whose trajectories diverge linearly, we expect an asymptotically logarithmic growth of $S$.

In the following sections, we shall investigate a simple dynamical model that has a well documented chaotic behavior, and it will be seen that these guesses are qualitatively correct. That model involves a discrete time variable, rather than a continuous time, in order to make calculations simpler. Instead of the continuous time evolution (4), there is then a unitary transformation of the components $c_n$ (explicitly given below).

II. THE TWIST AND TURN MAP

Consider a sequence of mappings of the unit sphere $x^2 + y^2 + z^2 = 1$, in which each step consists of a twist by an angle $a$ around the $z$-axis (namely, every $xy$ plane turns by an angle $a$), followed by a $90^\circ$ rigid rotation around the $y$-axis. The result of these consecutive twist and turn operations is

$$
x' = z,
$$

$$
y' = x \sin(a) + y \cos(a),
$$

$$
z' = -x \cos(a) + y \sin(a).
$$

(6)

This map is obviously area preserving. It was extensively investigated, both classically and in quantum mechanics, by Haake, Kuś and Scharf [6] who called it a “kicked top.” (It is not really like the motion of a rigid top, because of the torsion.) For low values of $a$, most classical orbits are regular (that is, they are quasi-periodic). As $a$ increases, so does the fraction of chaotic orbits, until for $a = 3$ most of the sphere is visited by a single chaotic orbit, as may be seen in Fig. 1. That figure also shows the presence of “forbidden” areas, corresponding to regular regions located around fixed points of the map [7]. All the following calculations refer to the case $a = 3$, unless stated otherwise.

The map (6) has interesting symmetries. Given any closed orbit, another closed orbit can be obtained by changing the signs of both $x$ and $z$. This symmetry will be called
$R_y$ (it is a rotation by $180^\circ$ around the $y$-axis). Moreover, for any pair of distinct orbits related by $R_y$, it is possible to obtain a third orbit (of twice the length) by means of a $180^\circ$ rotation of that pair of orbits around the $x$-axis. These symmetries have important consequences for the classification of Liouville densities, as will be seen in the next Section.

A characteristic property of each orbit is its Lyapunov exponent. In the present case, it may be defined as follows: consider an infinitesimal circle drawn on the sphere around the initial point of a fiducial orbit. As the map proceeds, this infinitesimal circle is deformed into an infinitesimal ellipse, having the same area. The ellipse rotates and stretches or contracts in an “erratic” way at each step. Let $a_n$ be the length of its semi-major axis after $n$ steps. The Lyapunov exponent (per step) is defined as

$$
\lambda = \lim_{n \to \infty} \frac{\log(a_n/a_0)}{n}.
$$

Such a limit indeed exists for a generic chaotic orbit [8, 9]. In the special case of a regular orbit, the pulsations of the ellipse are bounded, and therefore $\lambda = 0$.

We have computed in this way the Lyapunov exponents for $10^5$ orbits with randomly chosen initial points. Each orbit was terminated after $10^4$ steps (this usually happened when the orbit was regular), or, for chaotic orbits, when the major axis of the ellipse exceeded $10^{16}$ (because of the inevitable loss of precision in any further computation). The details of the calculations are given in Appendix A, and the results are displayed in Fig. 2. About 14% of the orbits are regular. For the chaotic ones, we obtained:

$$
\lambda = 0.346 \pm 0.071 \quad \text{(average} \pm \text{standard deviation)}.\tag{8}
$$

Ideally, $\lambda$ should have had a sharp value, the same for all chaotic orbits. This dispersion free value could in principle have been found by more sophisticated methods [10], but it was not needed for our present purpose.
III. MAPPING OF LIOUVILLE DENSITIES

Instead of considering individual orbits, that is, mapping of points into points, a more general approach, which gives new and instructive insights, is the mapping of Liouville densities. Let us imagine that an infinitesimal “mass” $\rho \, dA$ (which may be positive or negative) is attached to each area $dA$. Let us further assume that this mass is conserved during the twists and turns of the unit sphere, so that its density $\rho$ obeys the linear law

$$\rho'(x', y', z') = \rho(x, y, z),$$

by virtue of $dA' = dA$. Note that, as the mapping (6) is continuous, nearby points are mapped into nearby points, so that a blob is always mapped into a single blob (never into several disjoint blobs).

For the twist and turn map (6), these Liouville densities may belong to three invariant symmetry classes, according to their behavior under $R_y$ and $R_x$ (namely, 180° rotations around the $y$- and $x$-axes, respectively). For example, if $\rho = F(x^2, y^2, z^2, xyz)$ is a single valued function of its four arguments, this $\rho$ is even under $R_y$ and $R_x$, and is mapped by Eq. (9) into another function of the same type. Likewise, any $\rho = yF(x^2, y^2, z^2, xyz)$ is even under $R_y$ and odd under $R_x$, and is mapped by (9) into a function of the same type. For instance, the function $\rho = y$ has this property, because

$$y \rightarrow y' = x \sin(az) + y \cos(az) = y \left[ \cos(az) + \frac{xyz \, \sin(az)}{y^2} \right].$$

In general, any $\rho(x, y, z)$ can be written as the sum of three terms, belonging to one of the symmetry classes listed in Table 1.
Table 1. Symmetry classes of Liouville functions.

| $R_y$ | $R_x$ | Functional form |
|-------|-------|-----------------|
| even  | even  | $\rho = F(x^2, y^2, z^2, xyz)$ |
| even  | odd   | $\rho = yF(x^2, y^2, z^2, xyz)$ |
| odd   | $xF_1(x^2, y^2, z^2, xyz) + zF_2(x^2, y^2, z^2, xyz)$ |

A natural way of expanding Liouville functions on the unit sphere is the use of spherical harmonics,

$$\rho(\theta, \phi) = \sum_{lm} C_{lm} Y_{lm}^m(\theta, \phi),$$  \hspace{1cm} (11)

where the angles $\theta$ and $\phi$ are related to the cartesian coordinates in Eq. (6) in the usual way: $x = \sin \theta \cos \phi$, etc.

We shall use the common (but not universal) sign conventions [11, 12]

$$Y_{lm}^m(\theta, \phi) = \left[ \frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!} \right]^{1/2} \left( -1 \right)^m \cos^m \phi \, \sin \theta \, e^{im\phi} \, P_{lm}(\cos \theta),$$ \hspace{1cm} (12)

$$Y_{lm}^{-m}(\theta, \phi) = (-1)^m Y_{lm}^{m*}(\theta, \phi),$$

where $m \geq 0$ and $P_{lm}(\cos \theta)$ are the associated Legendre polynomials. The $Y_{lm}^m(\theta, \phi)$ are orthonormal, so that

$$C_{lm} = \int Y_{lm}^{m*}(\theta, \phi) \, \rho(\theta, \phi) \, d\Omega,$$ \hspace{1cm} (13)

where $d\Omega = \sin \theta \, d\theta \, d\phi$. In particular, the total mass, namely $\int \rho d\Omega = \sqrt{4\pi} C_{00}$, is constant for our area-preserving map. We shall henceforth ignore the trivial $C_{00}$ component and consider only the entropy of the other ones.

The nontrivial $C_{lm}$ transform as follows: during a twist, $\theta$ is constant, and

$$\phi \rightarrow \phi' = \phi + a \cos \theta.$$ \hspace{1cm} (14)

We thus have $\rho'(\theta, \phi + a \cos \theta) = \rho(\theta, \phi)$, or

$$\rho'(\theta, \phi) = \rho(\theta, \phi - a \cos \theta).$$ \hspace{1cm} (15)
whence

\[ C'_{jm} = \int Y_j^{m*}(\theta, \phi) \rho(\theta, \phi - a \cos \theta) \, d\Omega, \]  

(16)

because \( d\Omega' = d\Omega \). Substitution of (11) into (16) then gives

\[ C'_{jm} = \sum_l U^{(m)}_{jl} C_{lm}, \]  

(17)

where the \( U^{(m)}_{jl} \) are components of a unitary matrix:

\[ U^{(m)}_{jl} = \int Y_j^{m*}(\theta, \phi) Y_l^m(\theta, \phi) e^{-ima \cos \theta} \, d\Omega. \]  

(18)

An accurate method for computing \( U^{(m)}_{jl} \) for large \( j \) and \( l \) is described in Appendix B.

We thus see that a twist leaves \( m \) invariant but it introduces all the \( l \geq |m| \) (with exponentially small coefficients for large \( l \)), while a rotation mixes different \( m \) but leaves \( l \) invariant. This emergence of higher and higher \( l \) occurs only in the classical twist and turn map, which thus behaves in a quite different way from the corresponding quantum map [6, 7]. This is because in quantum theory \( l \) has the meaning of total angular momentum, and the latter is a constant of the motion under a twist (which is generated by \( J_2^2 \)), while the classical \( l \) has no such dynamical meaning and therefore need not be conserved.

Note that a pure twist is a regular motion: all the orbits are closed circles around the \( z \)-axis. We examined the growth of \( S \), as a function of a continuous twist angle \( a \), for two maps starting with \( \rho \) proportional to \( x \) (odd symmetry class) or to \( y \) (even-odd symmetry). These are represented by initial states with

\[ C_{11} = \mp C_{1,-1} = 1/\sqrt{2}, \]  

(19)

respectively, and all other \( C_{lm} = 0 \). Since different values of \( m \) do not mix during a twist, the \( D \)-entropy is the same in both cases. Figure 3 shows the result: the growth of \( e^S \) is roughly linear, as expected.
We now turn our attention to the rotations of the unit sphere. With spherical harmonics used as a basis, the matrix representation of a 90° rotation is well known [13, 14]: the index $l$ is not affected, and for each $l$ the $(2l + 1)$ components indexed by $m$ undergo a unitary transformation. Appendix B explains how to construct accurately these unitary matrices (we proceeded up to $l = 500$).

We checked the accuracy of our numerical calculations by verifying that unitarity held at each step, with an error less than $10^{-8}$. To achieve this result, we had to use a range of values of $l$ that increased by more than a factor 3 at each step. We thus had, at the fifth step, components $C_{lm}$ with $l$ up to 500. This implied that the rotation matrices had all possible odd orders up to 1001, and twist matrices had all orders up to 500. The next step would have exceeded the capacity of our computer (or entailed a severe loss of accuracy).

Figure 4 shows how $S$ grows with the number of steps. In the case $a = 3$, we considered two different initial Liouville densities, given by Eq. (19). These functions, which belong to different symmetry classes, turn out to have roughly linear rates of growth of their $D$-entropies, as expected, but, surprisingly, these rates are manifestly different from each other. We must therefore conclude that the growth of the $D$-entropy, contrary to the Kolmogorov-Sinai entropy [8, 9], is not related in a simple way to the Lyapunov exponents of individual orbits, because generic aperiodic orbits have no symmetry.

We also performed similar calculations for some lower values of $a$. For $a = 2$, the twist and turn map is mostly regular, but there still are small chaotic regions [6]. These chaotic regions become almost invisible for $a = 1.5$ or less. We thus expected to find a growth of $S$ starting about logarithmically, as for regular systems, and gradually becoming linear, with a small slope, due to the presence of small chaotic regions. However it turned out, as Fig. 4 shows, that for these low values of $a$ the growth of $S$ is not uniform. Rather, $S$ oscillates about a slowly increasing average. It is therefore hopeless to detect a clear transition from the logarithmic regime to the linear one, and we did not proceed further in these numerical simulations. (We also found oscillations for $a = 3$, when we started
with an unsymmetrized $f$, for example with $C_{11} = 1$, and all other $C_{lm} = 0$.

IV. CONCLUDING REMARKS

We found some results that were not unexpected, but we also had several surprises for which we can offer no explanation, and which may perhaps be worth further investigation. There can be no doubt that, for a given Liouvillian, the rate of growth of the $D$-entropy depends on the symmetry class of the Liouville density. Therefore, contrary to the Kolmogorov-Sinai entropy [8, 9], the $D$-entropy is not directly related to the Lyapunov exponent of classical trajectories.

Even more surprising is a quantitative comparison of Figures 3 and 4. The growth of $S$ for a pure twist (which is a regular mapping) is faster than its growth for a weakly chaotic twist and turn map (with low $a$), when we compare the total twist angle in the first case, and the sum of discontinuous twists of the discrete map.

The initial motivation of this work was a search for the existence of genuine quantum chaos (namely, phenomena that are not only a quantum simulation of classically chaotic properties). We have found definite clues that quantum chaos may indeed appear if, and only if, the quantum system is unbounded and has a continuous spectrum.

ACKNOWLEDGMENT

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APPENDIX A. THE LYAPUNOV EXPONENT

Consider infinitesimal deviations $x \rightarrow x + \epsilon \xi$, $y \rightarrow y + \epsilon \eta$, and $z \rightarrow z + \epsilon \zeta$, from a fiducial orbit of the map (6). These deviations satisfy

$$x \xi + y \eta + z \zeta = 0,$$

so as to lie on the surface of the sphere. We can also define the tangential components of the vector $(\xi, \eta, \zeta)$, namely

$$u = (-y \xi + x \eta) / \sqrt{1 - z^2} \quad \text{and} \quad v = \zeta / \sqrt{1 - z^2},$$

(21)
in the “east” and “north” directions, respectively.

Likewise, at the next step, let $x' \rightarrow x' + \epsilon \xi'$, etc. Neglecting terms of order $\epsilon^2$ and higher, we obtain from Eq. (6),

$$\xi' = \zeta,$$

$$\eta' = \xi \sin(az) + \eta \cos(az) - \zeta az',$$

$$\zeta' = -\xi \cos(az) + \eta \sin(az) + \zeta ay'.$$

(22)

This set of equations is the linear dynamical law for the evolution of the vector $(\xi, \eta, \zeta)$. We now want to know how an infinitesimal “unit” circle, namely a set of points with initial components $u = \cos \alpha$, $v = \sin \alpha$ (where $\alpha$ runs from 0 to $2\pi$), transforms into an ellipse (with the same area). The asymptotic growth of the major axis of this ellipse gives the Lyapunov exponent, as defined by Eq. (7).

To find how this infinitesimal circle transforms, we note that, by virtue of the linearity of (22), if the initial components of a tangential vector are $(\cos \alpha)$ and $(\sin \alpha)$, these components become, after a number of steps, $(T_{11} \cos \alpha + T_{12} \sin \alpha)$ and $(T_{21} \cos \alpha + T_{22} \sin \alpha)$, respectively, where the coefficients $T_{pq}$ are independent of $\alpha$. It is therefore enough to
consider two infinitesimal tangent vectors having, initially, $\alpha = 0$ and $\pi/2$. Their evolution determines all the components of $T_{pq}$, and the length of the semi-major axis is then obtained by maximizing the expression

$$r^2(\alpha) = (T_{11} \cos \alpha + T_{12} \sin \alpha)^2 + (T_{21} \cos \alpha + T_{22} \sin \alpha)^2,$$

as a function of $\alpha$. The result after $n$ steps is

$$a_n = [\sigma + (\sigma^2 - 1)^{1/2}]^{1/2},$$

where $\sigma = \sum_{pq} (T_{pq})^2$. Finally, the Lyapunov exponent is given by Eq. (7), in the limit $n \to \infty$.

APPENDIX B. THE TWIST MATRIX

The evaluation of the matrix elements $U_{jl}^{(m)}$ in Eq. (18) is the procedure which consumes most of the time in our calculations. Each one of the indices, $j, l, m$, may run up to 500. There are therefore many millions of different integrals for which no analytic expression is known. These integrals are, for large values of their indices, rapidly varying functions of $\cos \theta$, and a straightforward numerical integration, with the level of accuracy that we wanted, would be prohibitive.

We took advantage of the fact that a twist by a finite angle $a$ can be generated by a sequence of infinitesimal twists by an angle $\epsilon$, for which we can replace $e^{-im\epsilon z}$ by $(1-i m \epsilon z)$. This entails no loss of precision if $m \epsilon < 10^{-16}$, when we compute with 16 significant digits. The matrix elements $U_{jl}^{(m)}(\epsilon)$ can be evaluated explicitly (see below), and each matrix is then raised to the appropriate power. For example, by taking $\epsilon = 2^{-k} a$, we merely have to compute $(\ldots ((U^2)^2) \ldots)^2$, $k$ times.

We only explicitly need

$$\int Y_j^m *(\theta, \phi) Y_l^m (\theta, \phi) \cos \theta d\Omega = \text{const.} \times \int_{-1}^{1} P_j^m(z) P_l^m(z) z \, dz.$$  

(25)
This expression is readily evaluated by using the identity

$$z P_j^m(z) \equiv [(j - m + 1) P_{j+1}^m(z) + (j + m) P_{j-1}^m]/(2j + 1),$$  \hspace{1cm} (26)$$

and the orthogonality relations for associated Legendre polynomials [15].

**APPENDIX C. THE ROTATION MATRIX**

There are explicit formulas for the unitary rotation matrices $R_{mn}^{(j)}$ [13, 14] However, when $j$ is large, these formulas are not convenient for numerical calculations, because each matrix element is given as the tiny algebraic sum of a large number of huge terms with opposite signs. Only a few elements with $m = \pm j$, or $m$ close to $\pm j$, can easily be obtained from the general formula.

A much more efficient way of obtaining the $R$ matrix for a $90^\circ$ turn around the $y$-axis is to use its very definition, namely $R^\dagger J_x R = J_z$, or

$$J_x R = R J_z.$$  \hspace{1cm} (27)$$

With the standard representation, namely $(J_z)_{m n} = m \delta_{m n}$ and $J_x$ real, this gives

$$[(j + m) (j - m + 1)]^{1/2} R_{m-1,n}^{(j)} + [(j + m + 1) (j - m)]^{1/2} R_{m+1,n}^{(j)} = 2n R_{m,n}^{(j)}.$$  \hspace{1cm} (28)$$

Let us therefore define, for each $j$ and $n$, a “vector” $V_m$ by

$$R_{m,n}^{(j)} = (-1)^{n-m} 2^j \left[ \frac{(j+m)! (j-m)!}{(j+n)! (j-n)!} \right]^{1/2} V_m.$$  \hspace{1cm} (29)$$

From the explicit formulas mentioned above [13, 14], it can be seen that all the components of $V_m$ are integers, and in particular $V_{-j} = 1$ and $V_{1-j} = 2n$. The recursion relation (28) thus becomes

$$(j - m + 1) V_{m-1} - 2n V_m + (j + m + 1) V_{m+1} = 0.$$  \hspace{1cm} (30)$$
(This equation also appeared as the last equation of ref. [7], unfortunately marred by a misprint. The calculations in ref. [7] were correct.)

Even with the simple recursion formula (30), it is not trivial to obtain all the $V_m$ for $j > 50$ (when using double precision floating point arithmetics), because the recursion is unstable and small numerical errors grow exponentially. We therefore performed this calculation \textit{exactly}, using integer arithmetics; and we checked that the resulting matrices were indeed unitary.
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Captions of figures

FIG. 1. Area-preserving projection of the hemisphere $y > 0$. The figure shows 20000 points belonging to a single chaotic orbit. The empty regions are filled by regular orbits, not shown here.

FIG. 2. Distribution of Lyapunov exponents for $10^5$ randomly chosen orbits. Each bin of the histogram has width $10^{-2}$.

FIG. 3. Growth of the $D$-entropy for a continuous twist, as a function of the twist angle.

FIG. 4. Growth of the $D$-entropy for the twist and turn map, for various values of the twist parameter $a$. 