Quantum Mechanical Tools in Applications to Classical Dynamical Systems

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A recently developed approach to classical and quantum dynamical entropy involving generalized partitions of unity allows one to use the mathematical formalism typical for quantum statistical mechanics to analyze classical dynamical systems. In particular, density matrices, their von Neumann entropy, and irreversible quantum dynamical maps corresponding to measurement processes appear. To illustrate the power of this new technique we give a simple proof of the Ruelle's inequality between the Kolmogorov-Sinai entropy and the Lyapunov exponents. Continuous time classical dynamical systems are briefly discussed also. [S0031-9007(98)07034-3]

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In this Letter we discuss mostly conservative, discrete time classical dynamical systems described by a triple $(X, d\mu, \Phi)$ where $d\mu$ denotes a probability measure on the phase space X and $\Phi : X \mapsto X$ is a measure preserving dynamical map. Koopman's formalism [1] allows us to describe $(X, d\mu, \Phi)$ in terms of "quantumlike objects": the Hilbert space $L^2(X, d\mu)$ of square integrable functions with the scalar product $\langle f, g\rangle = \int f^*(x) g(x)\, d\mu(x)$ and the unitary operator

$$(Uf)(x) = f(\Phi(x)), \qquad f \in L^2(X, d\mu). \tag{1}$$

The analysis of spectral properties of U is one of the basic topics in the classical ergodic theory [2]. The recently developed approach to dynamical entropy of classical and quantum systems adds new ideas and techniques to Koopman's formalism. In particular, the notion of density matrix and completely positive maps which are used in quantum statistical mechanics to describe the dynamics of an open system interacting with an environment or being subject to a measurement process will find classical applications. One should stress here that the quantum systems which appear in this approach are fictitious ones with no direct physical connection to the original classical system. The main idea is to use the mathematical formalism and experience gained in quantum physics to solve the problems of classical ergodic theory.

We begin with the notion of a density matrix ρ which is a trace class positive and normalized ($\mathrm{tr}\rho = 1$) operator acting on the Hilbert space of the quantum system and describing a mixed state of the system. The average value of the observable given by a self-adjoint operator $A = A^\dagger$ at the state ρ reads $\langle A\rangle = \mathrm{tr}(\rho A)$. Denoting the (possibly degenerated) eigenvalues of ρ by $\{\lambda_j\}$ we can calculate the von Neumann entropy $S[\rho]$ of the density matrix ρ as

$$S[\rho] = -\sum_j \lambda_j \ln \lambda_j = -\mathrm{tr}(\rho \ln \rho). \tag{2}$$

An irreversible (non-Hamiltonian) dynamical map for the open quantum system interacting with an environment and particularly with a measuring apparatus is given by a completely positive linear transformation acting on density matrices (Schrödinger picture) and represented in the form

$$\rho \mapsto \Lambda(\rho) = \sum_\alpha W_\alpha \rho W_\alpha^\dagger, \tag{3}$$

with $\sum W_\alpha^\dagger W_\alpha = \mathbf{1}$. These dynamical maps can transform pure states into mixed ones and change the entropy of a state. Discrete time open quantum systems are described by the powers of the single dynamical map $\{\Lambda^n; n \in \mathbf{N}\}$ which form a discrete time dynamical semigroup. For continuous time irreversible dynamical systems we use quantum Markovian master equations of the form

$$\frac{d\rho_t}{dt} = L\rho_t; \qquad t \geq 0, \tag{4}$$

with the standard (Lindblad-Gorini-Kossakowski-Sudarshan) form of the generator [3]

$$L\rho = -i[H, \rho] + \frac{1}{2}\sum_\beta \{[V_\beta, \rho V_\beta^\dagger] + [V_\beta \rho, V_\beta^\dagger]\}, \tag{5}$$

where $H = H^\dagger$ is a Hamiltonian of the system.

In our special case of the Hilbert space $L^2(X, d\mu)$ a density matrix ρ is given by a positively defined integral kernel $\rho(x|y)$ satisfying the normalization condition $\int \rho(x|x)\, d\mu(x) = 1$ and its spectral decomposition becomes

$$\rho(x|y) = \sum_j \lambda_j \psi_j(x) \psi_j^*(y), \tag{6}$$

with

$$\int_X \psi_i^*(x)\psi_j(x)\, d\mu(x) = \delta_{ij}, \qquad \lambda_j > 0,$$

$$\sum_j \lambda_j = 1. \tag{7}$$

In the standard approach to the Kolmogorov-Sinai entropy the fundamental object is a finite partition of X into disjoint subsets $C = \{C_1, C_2, \dots, C_k\}$. There exists a corresponding family of indicator functions denoted by the

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same symbol $C = \{\chi_{C_1}, \chi_{C_2}, \dots, \chi_{C_k}\}$ where $\chi_C(x) = 1$ for $x \in C$; $\chi_C(x) = 0$ for $x \notin C$. The partition C produces the density matrix

$$\rho_C(x|y) = \sum_{j=1}^{k} \chi_{C_j}(x)\chi_{C_j}(y). \tag{8}$$

As the functions χ_{C_j} are mutually orthogonal and $\|\chi_{C_j}\| = \sqrt{\mu(C_j)}$ the eigenvalues of ρ_C are equal to $\{\mu(C_j); j = 1, \dots, k\}$ and the von Neumann entropy of ρ_C is equal to the standard entropy of the partition

$$S[\rho_C] = -\sum_{j=1}^{k} \mu(C_j) \ln \mu(C_j). \tag{9}$$

The main idea of the theory developed in [4–6] is to replace partitions of the phase space X by the "operational partitions of unity" which consist of elements of the algebra of bounded (complex) observables of a classical or quantum dynamical system. This approach was designed for the analysis of infinite quantum systems; nevertheless, it was successfully applied for the discussion of "quantum chaos" in finite quantum systems [7] and in the classical domain also [6]. In the case of a classical dynamical system an operational partition of unity is simply a family $\mathcal{F} = \{f_1, f_2, \dots, f_k\}$ of complex-valued functions, $f_j : X \mapsto \mathbf{C}$ satisfying the normalization condition

$$\sum_{j=1}^{k} |f_j(x)|^2 = 1. \tag{10}$$

The density matrix $\rho_{\mathcal{F}}$ associated with the partition of unity $\mathcal{F}$ is defined as

$$\rho_{\mathcal{F}}(x|y) = \sum_{j=1}^{k} f_j(x) f_j^*(y). \tag{11}$$

Such density matrices have additional properties

$$\rho(x|x) = 1, \qquad |\rho(x|y)| \le 1. \tag{12}$$

Generally, the functions f_j are not orthogonal and the computation of the entropy $S[\rho_{\mathcal{F}}]$ involves the solution of the eigenvalue problem for $\rho_{\mathcal{F}}$.

The dynamical map Φ enters the game when we introduce the time-dependent density matrices $\rho_{\mathcal{F}}^{(n)}$ which possess again the structure given by Eq. (11),

$$\begin{aligned} \rho_{\mathcal{F}}^{(n)}(x|y) &= \prod_{m=0}^{n-1} \rho_{\mathcal{F}}(\Phi^m(x)|\Phi^m(y)) \\ &= \sum_{j_1, j_2, \dots, j_n} f_{j_1}(x) f_{j_2}(\Phi(x)) \cdots f_{j_n}(\Phi^{n-1}(x)) \\ &\quad \times f_{j_1}^*(y) f_{j_2}^*(\Phi(y)) \cdots f_{j_n}^*(\Phi^{n-1}(y)). \end{aligned} \tag{13}$$

The family of density matrices $\{\rho_{\mathcal{F}}^{(n)}\}$ can be seen as obtained by applying a certain, discrete time, completely positive dynamical semigroup $\{\Lambda^n; n = 0, 1, 2, \dots\}$ to the initial pure state $|\xi\rangle\langle\xi|, \xi(x) \equiv 1$. One can explicitly compute the action of Λ, which is a special case of the dynamical map given by (3)

$$\Lambda(\rho) = \sum_{j=1}^{d} \hat{f}_j U \rho U^\dagger \hat{f}_j^\dagger, \qquad \rho_{\mathcal{F}}^{(n)} = \Lambda^n(|\xi\rangle\langle\xi|), \tag{14}$$

where $\hat{f}$ is the multiplication operator by the function f and U is given by Eq. (1). The time evolution $\{\Lambda^n; n = 0, 1, 2, \dots\}$ is an irreversible one, increases always the entropy and can be interpreted as an effect of a "fuzzy position repeated measurements" [8] performed at discrete times on the fictitious quantum system with the dynamics given by the unitary operator U.

The dynamical entropy $h[\mathcal{F}]$ of the partition of unity $\mathcal{F}$ is an asymptotic entropy production per a single evolution step, i.e.,

$$h[\mathcal{F}] = \lim_{n \to \infty} \frac{1}{n} S[\rho_{\mathcal{F}}^{(n)}]. \tag{15}$$

It is easy to check that in the case of a partition of unity given by the indicator functions $\{\chi_{C_j}\}$ we obtain again the standard dynamical entropy of the partition $\{C_j\}$ of X. The following result can be proved using the results of [6].

Theorem.—For the dynamical system $(X, d\mu, \Phi)$

$$h_{\mathrm{KS}} = \sup_{\mathcal{F}} h[\mathcal{F}], \tag{16}$$

where h_{KS} is a Kolmogorov-Sinai entropy and the supremum is taken over all partitions of unity.

Obviously, it follows from the very definition of the Kolmogorov-Sinai entropy that it is enough to take the supremum over partitions consisting of indicator functions. On the other hand, taking the supremum over all generalized partitions is practically useless. Therefore it is necessary to strengthen the above theorem by taking the supremum over certain restricted classes of functions. It has been done in [6] where a rather technical notion of *H-dense* subalgebras has been introduced. As a consequence it has been proved that taking a supremum in the right-hand side of Eq. (16) over partitions of unity consisting of functions from a H-dense subalgebra we obtain the Kolmogorov-Sinai entropy of the system $(X, d\mu, \Phi)$.

The following examples of H-dense subalgebras of real or complex-valued functions appear in applications: (a) stepwise functions; (b) continuous functions; (c) infinitely differentiable (smooth) functions; (d) polynomials of a given set of generating functions.

The example of the Arnold cat map studied in [6] shows that using partitions of unity of the type (d) one can simplify the computation of the dynamical entropy. In the following we would like to show that smooth partitions (c) introduce new useful analytical techniques into the classical ergodic theory.

Consider a smooth ergodic dynamical system with a compact ν-dimensional manifold X. In a local coordinate system the dynamical map $x' = \Phi(x)$ is given by a set of equations

$$x'^k = \phi^k(x^1, x^2, \dots, x^\nu). \tag{17}$$

The chaotic properties of such a system are characterized by the Lyapunov exponents. To define them we consider a Riemannian metric on X given by the metric tensor $g_{rs}(x)$. The infinitesimal distance δl between two points is given by $(\delta l)^2 = g_{rs}(x)\delta x^r \delta x^s$ and changes in time according to

$$(\delta l)^2(m) = \frac{\partial \phi^p_{(m)}(x)}{\partial x^r}\, g_{pq}(\Phi^m(x))\, \frac{\partial \phi^q_{(m)}(x)}{\partial x^s}\, \delta x^r \delta x^s, \tag{18}$$

where we apply the following notation for the powers of the dynamical map

$$x'_{(m)} = \Phi^m(x), \qquad x'^k_{(m)} = \phi^k_{(m)}(x^1, x^2, \ldots, x^\nu). \tag{19}$$

Depending on the direction of the vector δx^r the distance $\delta l(m)$ increases or decreases according to the exponential law $\sim\exp \lambda_p m$, where $\{\lambda_p; p = 1, 2, \ldots, \nu\}$ is a set of Lyapunov exponents which are independent on the metric g_{rs} and x [9].

As we are looking for the relations between the Lyapunov exponents and the Kolmogorov-Sinai entropy we take a fixed partition $\mathcal{F}$ which consists of smooth real functions. Because of the property (12) we can always write putting $\rho^{(n)}_{\mathcal{F}} \equiv \rho^{(n)}$

$$\frac{\partial}{\partial y^r}\, \rho^{(1)}(x|y)_{y=x} = 0, \tag{20}$$

$$-\frac{\partial^2}{\partial y^r \partial y^s}\, \rho^{(1)}(x|y)_{y=x} = g_{rs}(x), \qquad [g_{rs}(x)] \geq 0, \tag{21}$$

with a positively defined real-valued matrix $[g_{rs}(x)]$. In the following we shall use it as a Riemannian metric on X, and therefore we can keep the same notation as in (18). After a straightforward computation we obtain

$$\begin{aligned} A^{(n)}_{rs}(x) &= -\frac{\partial^2}{\partial y^r \partial y^s}\, \rho^{(n)}(x|y)_{y=x} \\ &= \sum_{m=0}^{n-1} \frac{\partial \phi^p_{(m)}(x)}{\partial x^r}\, g_{pq}(\Phi^m(x))\, \frac{\partial \phi^q_{(m)}(x)}{\partial x^s}. \end{aligned} \tag{22}$$

Our first goal is to calculate the mean value of the following self-adjoint operator acting on $L^2(X, d\mu)$

$$H^{(n)} = -\tfrac{1}{4}\,([A^{(n)}(x)^{-1}]^{rs}\partial_r\partial_s + \text{H.c.}) \tag{23}$$

in the quantum state given by the density matrix $\rho^{(n)}$. From Eqs. (22) and (23) it follows that

$$\text{tr}(\rho^{(n)} H^{(n)}) = \nu/2. \tag{24}$$

The next step is to estimate $\lim_{n\to\infty} \frac{1}{n} \log(\det[A^{(n)}(x)])$. Taking into account the structure of the matrix $[A^{(n)}(x)]$ (22), we see that the product of its eigenvalues is dominated (up to a multiplicative constant) by a product of $\exp\{2\lambda_p n\}$ with $\lambda_p > 0$ corresponding to "stretching directions." Therefore

$$\lim_{n\to\infty} \frac{1}{n}\, \ln(\det[A^{(n)}]) \leq 2 \sum_{p;\lambda_p>0} \lambda_p. \tag{25}$$

To prove the Ruelle's inequality [10], we construct the density matrix $\delta^{(n)}$ which maximizes the entropy under the condition

$$\text{tr}(\delta^{(n)} H^{(n)}) = \nu/2. \tag{26}$$

The structure of $\delta^{(n)}$ is the following:

$$\delta^{(n)} = Z^{-1} \exp(-\beta H^{(n)}). \tag{27}$$

The density matrix $\delta^{(n)}$ describes the quantum equilibrium state (at the inverse temperature β) of the particle with the configuration space X and the classical Hamiltonian $\mathcal{H} = \frac{1}{2}[A^{(n)-1}]^{rs} p_r p_s$. Consider for simplicity the one dimensional case of a quantum particle on an interval $[0, L]$ with the classical Hamiltonian $\mathcal{H}_1 = p^2/2m$. For large values of the mass m the semiclassical approximation will be valid, and the quantum entropy $S_q[\beta]$ of the equilibrium state at the inverse temperature β can be written as

$$\begin{aligned} S_q[\beta] &= S_{cl}[\beta] + o(1/m), \\ S_{cl}[\beta] &= \tfrac{1}{2}\ln(2\pi m) + \ln L - \tfrac{1}{2}\ln\beta + \tfrac{1}{2}, \end{aligned} \tag{28}$$

where $S_{cl}[\beta]$ is the classical entropy for this model.

As we are computing $\lim_{n\to\infty}(1/n)S(\delta^{(n)})$, then according to Eq. (28) the nontrivial contributions come from the degrees of freedom corresponding to the eigenvalues of $A^{(n)}$ which grow exponentially with n. For such a case all quantum and finite volume corrections do not contribute to the final result, the classical counterpart of the condition (26) gives $\beta \approx 1$, and the leading term for the entropy is obtained from the classical expression for the free particle with the "mass matrix" $A^{(n)}$

$$S(\delta^{(n)}) \approx \tfrac{1}{2}\ln(\det A^{(n)}). \tag{29}$$

Combining now the inequality (25), the estimation (29), and the fact that $S(\rho^{(n)}) \leq S(\delta^{(n)})$, we obtain

$$\lim_{n\to\infty} \frac{1}{n}\, S(\rho^{(n)}) \leq \sum_{p;\lambda_p>0} \lambda_p. \tag{30}$$

As by a proper choice of the smooth partition $\mathcal{F}$ we can approach the supremum in (13), we obtain the Ruelle's inequality

$$h_{\text{KS}} \leq \sum_{p;\lambda_p>0} \lambda_p. \tag{31}$$

The standard definition of the dynamical entropy is given for discrete time dynamical systems. To apply it for continuous time dynamics $\{\Phi_t; t \in \mathbf{R}\}$ we have to introduce a time step τ, calculate the Kolmogorov-Sinai entropy for the corresponding dynamical map Φ_τ, and then using the property $h_{\text{KS}}(\Phi^n) = |n| h_{\text{KS}}(\Phi)$ we may define $h_{\text{KS}} = h_{\text{KS}}(\Phi_\tau)/\tau$. We shall see that the presented approach enables us to avoid the procedure of discretization.

Consider a continuous time dynamical systems (X, dx, Φ_t) given by the equations of motion

$$\frac{dx_t^r}{dt} = \Gamma^r(x_t), \qquad x_t = \Phi_t(x), \tag{32}$$

with the measure (volume) preservation condition $\partial_r \Gamma^r = 0$. Instead of a discrete time dynamical semigroup $\{\Lambda^n, n = 0, 1, \ldots\}$ given by (14), we use the completely positive dynamical semigroup [3] describing "continuous time fuzzy position measurement" [8] and governed by the following Markovian master equation which is a particular case of (4) and (5) with self-adjoint V_β:

$$\frac{d\rho_t}{dt} = -i[K, \rho_t] - \frac{1}{2} \sum_j [\hat{w}_j, [\hat{w}_j, \rho_t]]. \tag{33}$$

Here $K = i\Gamma^r(x)\partial_r$ is the generator of the unitary Koopman's evolution ("quantum Hamiltonian") and $\hat{w}_j$ denotes the multiplication operator by the real function $w_j(x)$. Applying Trotter's product formula and using explicit expressions, we can easily find the solution of (33) with the initial condition $\rho_0(x|y) = 1$,

$$\rho_t(x|y) = \exp\left\{-\frac{1}{2} \sum_j \int_0^t [w_j(x_s) - w_j(y_s)]^2 \, ds\right\}, \quad t \geq 0. \tag{34}$$

We can define now the dynamical entropy of the stochastic perturbation $\mathbf{W} = (w_1, w_2, \ldots, w_l)$ as

$$h[\mathbf{W}] = \lim_{t \to \infty} \frac{1}{t} S[\rho_t]. \tag{35}$$

The supremum of $h[\mathbf{W}]$ over a large enough class of stochastic perturbations is expected to be equal to the Kolmogorov-Sinai entropy defined in a standard way. Repeating our analysis of above one can easily prove that this supremum is not larger than the sum of positive Lyapunov exponents.

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