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HOW TO GENERALIZE THE LAPUNOV EXPONENT FOR QUANTUM MECHANICS

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1. INTRODUCTION

Chaos in classical dynamics may be defined as exponential increase of the distance $d(t)$ between two neighboring trajectories in the phase space, or quantitatively, as positiveness of the largest Lapunov exponent λ_c of the system. In the simplest case

$$\lambda_c = \lim_{t\to\infty} \lambda(t); \qquad \lambda(t) = \lim_{d(0)\to 0} \frac{1}{t} \ln \frac{d(t)}{d(0)}. \tag{1}$$

Since the concept of trajectory looses its meaning in quantum mechanics, the above definition cannot be directly applied for quantum systems, and other approaches were proposed (Toda and Ikeda, 1985; Haake et al. 1992).

Our object is to extract from the time evolution of the quantum system the information whether the dynamics of the corresponding classical analogue is chaotic. Generalizing the concept of the Lapunov exponent λ_c for quantum mechanics one needs to find an appropriate meaning of the distance d_Q between two quantum states and has to discuss the sense of each of two limits in eq. (1).

2. INITIAL DISTANCE AND TIME LIMIT

Instead of the initially close points of the classical phase space we take in the quantum case two corresponding coherent states (Haake et al. 1992). The limit $d(0) \to 0$ in the definition (1) corresponds to the linearization of the classical dynamics. A similar procedure might be also applied in quantum mechanics, although there might be a large overlap between two close quantum states. On the other hand the limit $t \to \infty$, appropriate in classical mechanics, may not be applicable in the quantum case. It has been observed (Berman and Kolovsky 1983) that the wave packet follows the classical trajectory only up to a time τ of the order of $ln(\hbar)/\lambda_c$. On a larger time scale the distance between two arbitrary close quantum states may decrease due to quantum recurrences. To avoid this effect we take the temporal quantum exponent $\lambda_Q(t)$ at a finite time T_Q depending on $\hbar$ and the time behaviour of $\lambda(t)$. In the classical limit the time T_Q should tend to infinity.

3. DISTANCE BETWEEN QUANTUM STATES

For simplicity we shall analyze the case where the classical phase space S is a compact M-dimensional manifold. Let $|\alpha\rangle$ denote a coherent state defined for each point α belonging

to S. Any quantum state $|\Psi_i\rangle$ can be uniquely represented by the Husimi function (Takahashi, Saito 1985) also known as Q-representation: $Q_i(\alpha) = |\langle\Psi_i|\alpha\rangle|^2/\pi$. The problem of finding the distance d_Q between two quantum states is then equivalent to defining a metric ρ in the space $P(S)$ of all functions $Q_i : S \to R_+$ normalized by $\int Q_i(\alpha)d^M\alpha = 1$.
The metric ρ ideal for our purposes should posses the following properties:

A) ρ fulfills the axioms of a metric,

B) ρ generates the natural topology on $P(S)$,

C) ρ is isometrically invariant,

D) ρ possesses the appropriate classical limit, i.e., the distance between distributions representing two coherent states $|\alpha_1\rangle$ and $|\alpha_2\rangle$ tends to the Riemannian distance between two points α_1 and α_2 for $\hbar \to 0$,

E) ρ might be reasonably approximated by numerical calculations.

Note that accordingly to the definition (1) two relatively estimable metrics lead to the same value of the Lapunov exponent. Several different metrics are used to estimate the closeness between probability distributions (Rachev 1991), but it is not easy to find a suitable one satisfying conditions A) - E).

4. CANDIDATES FOR THE METRIC ρ

Let A be a measurable subset of S and let $Q_1(A)$ denote $\int_A Q_1(\alpha)d^M\alpha$. Consider

a) L^1 metric ρ_1

$$\rho_1(Q_1,Q_2) := \int_S |Q_1(\alpha) - Q_2(\alpha)|d^M\alpha, \tag{2}$$

b) Uniform (Kolomogorov) metric ρ_u

$$\rho_u(Q_1,Q_2) := \sup\left\{|Q_1(A) - Q_2(A)| : A \subset S\right\}. \tag{3}$$

These simplest metrics do not possess the required property D.

Let us define

c) Cumulant semimetric ρ_c

$$\rho_c^2(Q_1,Q_2) = \sum_{l=1}^{\infty} C_l \sum_{k=0}^{k=l} (\mu_{k,l-k}^{(1)} - \mu_{k,l-k}^{(2)})^2, \tag{4}$$

where $\mu_{k,l}^{(i)}$ are the cumulants of function $Q_i(\alpha)$ and $k,l = 0,1,2...$, (for simplicity we consider here a two dimensional space S). The coefficient $C_1 = 1$ and $\{C_l\}$ is a positive sequence ensuring the convergence of the above series. Note that in the classical limit all higher cumulants of coherent states vanish, so the metric ρ_c tends to the distance between two points in the phase space (condition D). On the other hand this quantity does not satisfy the axioms of a metric (there are different functions with ρ_c equal to zero) and may hardly be appropriate to describe correctly the complicated differences between two close coherent states evolving in the classically chaotic domain.

d) Monge-Kantorovich metric ρ_k

Consider the space $V = S \times R_+$ consisting of points $v = \{\alpha_1, ..\alpha_M, f\}$. Let Ω_i denote the set of all $v \in V : 0 \le f \le Q_i(\alpha)$. Due to normalization of Q_i the integral $\int_{\Omega_i} d^M\alpha df$ is equal to unity. Consider a transformation $T : V \to V$ and $\Omega_1 \to \Omega_2$. Let $v' = T(v)$. We shall look for a C^1 transformation T_k giving the minimal displacement integral and define (Rachev 1991)

$$\rho_k(Q_1, Q_2) := \inf \int_{\Omega_1} \sqrt{\sum_{m=1}^{M} (\alpha_m - \alpha'_m)^2} \; d^M\alpha \; df, \tag{5}$$

where the infimum is taken over all volume conserving transformations T. In a descriptive language, shoveling a pile of sand into a new location we minimalize the total path traveled by all grains.

The metric ρ_k fulfills the condition D and for one dimensional space $S = R$ the distance ρ_k is equal to (Rachev 1991)

$$\rho_k(Q_1, Q_2) = \int_{-\infty}^{+\infty} |F_1(\alpha) - F_2(\alpha)| d\alpha, \tag{6}$$

where $F_i(\alpha)$ stands for the distribuant $\int_{-\infty}^{\alpha} Q_i(x)dx$. The partial differential equations for the transformation T_k arising from the variational principle are complicated for two or higher dimensional space S and even numerical approximation of the distance ρ_k becomes difficult. As an example of a metric with properties A-D we suggest

e) Prokhorov metric ρ_p

$$\rho_p(Q_1, Q_2) := \inf \left\{ \epsilon > 0 : Q_1(A) \le Q_2(A^\epsilon) + \epsilon/\Delta \quad \text{for all closed} \quad A \subset S \right\}, \tag{7}$$

where Δ is the diameter of the compact set S and A^ϵ denotes ϵ-neighbourhood of the set A (Prokhorov 1956). Since in a general case an efficient numerical approximation of this distance is hardly possible we define

f) Simplified Prokhorov metric ρ_s

$$\rho_s(Q_1, Q_2) := \inf \big\{ \epsilon > 0 : Q_1(B(\alpha, r - \epsilon)) - \epsilon/\Delta \le Q_2(B(\alpha, r)) \le Q_1(B(\alpha, r + \epsilon)) + \epsilon/\Delta$$

$$\text{for all} \quad \alpha \in S, \quad r > 0 \big\}, \tag{8}$$

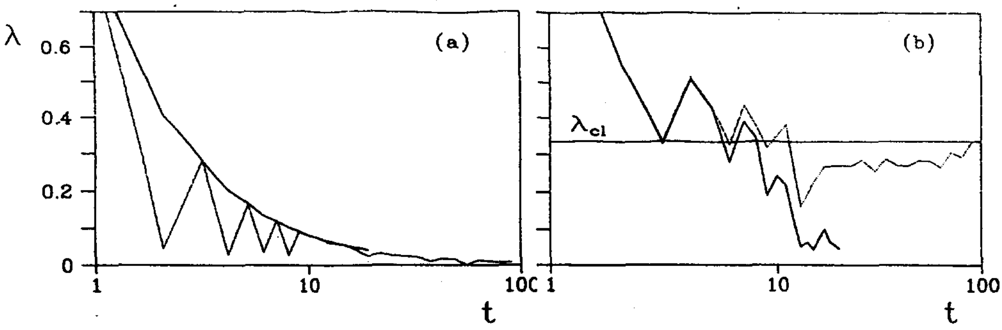
where $B(\alpha, r)$ stands for a circle of radius r with the center in the point α. The simplified metric ρ_s gives and upper estimation for ρ_p and might be easier implemented for numerical computation.

5. NUMERICAL RESULTS

As a model system we have chosen the periodically kicked top defined by the unitary evolution operator U (Haake at al. 1986)

$$U = \exp(-ikJ_x^2/2j)\exp(-i\pi J_z/2), \tag{9}$$

where J_x and J_z are the components of the angular momentum operator and the quantum number $j \sim \hbar^{-1}$ determines the size N of the matrix representation of U as $N = 2j + 1$. The dynamics of the corresponding classical system is regular for $k = 0$ and globally chaotic for $k > 6$. For an intermediate value $k = 3$ the regular domains coexist with chaotic layers.



The above figure presents the time dependence of the temporarily exponent $\lambda(t)$ obtained with $j = 2000$ and $k = 3.0$ for initial points located in a) regular island; and b) chaotic sea. The dotted line represents the classical calculation and its asymptotic shows the exact value of Lapunov exponent λ_c. The solid line is obtained in the quantum calculations based on the distances between the mean values of the states (the simplest cumulant semimetric ρ_c with $C_i = 0$ for $i \geq 2$). Even this crude tool allows to distinguish between two different kinds of the classical dynamics. Moreover, the numerical values of the quantum temporarily exponent taken at the time T_Q gives the correct order of magnitude of the classical Lapunov exponent (for the choice of T_Q see (Haake et al. 1992)).

6. CONCLUSION

The analysis of the time evolution of the mean values of the quantum wave packets enables to recognize the classically chaotic fragments of the phase space and to receive a rough estimation of the classical Lapunov exponents. Such results might be improved by measuring the distance between two quantum states with one of the sophisticated metrics d) - f), which are more suitable to detect the complicated structure of the coherent states evolving in a classically chaotic system.

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