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Quantum sensitive dependence

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Abstract

Wave functions of bounded quantum systems with time-independent potentials, being almost periodic functions, cannot have time asymptotics as in classical chaos. However, bounded quantum systems with time-dependent interactions, as used in quantum control, may have continuous spectrum and the rate of growth of observables is an issue of both theoretical and practical concern.

Rates of growth in quantum mechanics are discussed by constructing quantities with the same physical meaning as those involved in the classical Lyapunov exponent. A generalized notion of quantum sensitive dependence is introduced and the mathematical structure of the operator matrix elements that correspond to different types of growth is characterized. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Bounded classical systems that are chaotic, display exponential growth of initial perturbations and other interesting long-time asymptotics, like exponential decay of correlations. In contrast, quantum Hamiltonians of bounded systems with time-independent potentials, having discrete spectrum, their wave functions are almost periodic functions. For this reason the work on "quantum chaos" has shifted from consideration of long-time properties to the statistics of energy levels of quantum systems with a chaotic classical counterpart (for a review of recent work see [1] and references therein).

However, quantum systems with bounded configuration space but time-dependent interactions (for example, particles in an accelerator subjected to electromagnetic kicks or the systems used in quantum control) may have continuous spectrum. Therefore, the estimation and control of the rate of growth, of the perturbed matrix elements of observables, becomes an issue of both theoretical and practical concern.

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In classical mechanics the most important asymptotic indicator of chaotic behavior is the Lyapunov exponent (an ergodic invariant). Therefore, a natural first step to discuss rates of growth in quantum mechanics seems to be the construction of a quantum Lyapunov exponent. After a few heuristic attempts by several authors (see references in [2]) a satisfactory construction has been achieved [2], in the sense that the phase-space observables that are used are exactly the same in classical and quantum mechanics. It uses the tomographic formulation which describes conventional quantum mechanics by a set of marginal probability densities [3]. Then, the only difference between the classical and the quantum exponent lies in the time evolution dynamical equation. In Section 2 we recall this result. Translating it from tomographic densities to traces of operators, it turns out that the quantum Lyapunov exponent measures the rate of growth of the trace of position and momentum observables starting from a singular initial density matrix.

A positive Lyapunov exponent corresponds to exponential growth of these traces. However, the same quantities may serve to characterize other types of growth, leading to a generalized notion of quantum sensitive dependence.

There are examples where exponential rates of growth (as in classical chaos) are also found in quantum systems (Section 3). However, in many other cases, quantum mechanics seems to have a definite taming effect on classical chaos. Therefore, a generalized notion of quantum sensitive dependence, corresponding to rates of growth milder than exponential, might be of interest to classify different types of quantum complexity or to characterize the degree of accuracy achievable in quantum control.

Quantum sensitive dependence is discussed in Section 4, as well as the mathematical structure of the operator matrix elements, in the spectral representation of the trace, that corresponds to each type of growth. A convenient unified framework to discuss these matters is the space of ultradistributions of compact support and their Fourier images [4,5].

2. The quantum Lyapunov exponent

As a first step we will rewrite the results of Ref. [2] using operator traces. In Ref. [2] the quantum Lyapunov exponent along the phase-space vector $v = (v_1 v_2)$ is shown to be

$$\lambda_v = \lim_{t\to\infty} \frac{1}{t} \log \left\| \int d^n X\, d^n\mu\, d^n\nu\, e^{iX\bullet\mathbf{1}} \left(\begin{pmatrix} \nabla_\mu \\ \nabla_\nu \end{pmatrix} \delta^n(\mu)\delta^n(\nu) \right) M_t(X,\mu,\nu) \right\|, \tag{1}$$

where

$$M_t(X,\mu,\nu) = \int \Pi\left(X,\mu,\nu,X',\mu',\nu',t,0\right) M_0(X,\mu,\nu)\, dX'^n\, d\mu'^n\, d\nu'^n \tag{2}$$

is the time evolved tomographic density [3], starting from the initial condition

$$M_0\left(X',\mu',\nu'\right) = \left(\left(v_1 \circledast \mu' + v_2 \circledast \nu'\right) \bullet \nabla_{X'}\right)\delta^n\left(X' - \mu' q_0 - \nu' p_0\right), \tag{3}$$

$a \circledast b$ being defined as

$$(a \circledast b)_i = a_i b_i.$$

When Π is the classical propagator, λ_v, as defined in Eq. (1), coincides with the usual classical Lyapunov exponent constructed from the tangent map. The only difference between classical and quantum Lyapunov exponents lies in the dynamical law of the propagator, thus insuring that we are dealing with quantities with the same physical meaning.

For a system with Hamiltonian

$$H = \frac{p^2}{2} + V(q), \tag{4}$$

the evolution equation for the quantum propagator of the tomographic densities is

$$\frac{\partial \Pi}{\partial t} - \mu \bullet \nabla_\nu \Pi - \nabla_x V(\tilde{q}) \bullet (\nu \circledast \nabla_X \Pi) + \frac{2}{\hbar} \sum_{n=1}^{\infty} (-1)^{n+1} \left(\frac{\hbar}{2}\right)^{2n+1} \frac{\nabla_{i_1 \cdots i_{2n+1}} V(\tilde{q})}{(2n+1)!} (\nu \circledast \nabla_X)_{i_1} \cdots (\nu \circledast \nabla_X)_{i_{2n+1}} \Pi = 0 \tag{5}$$

with initial condition

$$\lim_{t \to t_0} \Pi(X, \mu, \nu, X', \mu', \nu', t, t_0) = \delta^n(X - X') \delta^n(\mu - \mu') \delta^n(\nu - \nu') \tag{6}$$

reducing for $\hbar = 0$ to the classical evolution equation.

In the tomographic formulation, classical and quantum mechanics are both described by a set of positive probability distributions $M_t(X, \mu, \nu)$, the $\hbar$-deformation appearing only in the time-evolution. It is this fact that allows the notion of Lyapunov exponent to be carried over without ambiguity from classical to quantum mechanics. However, to relate the Lyapunov exponent to the behavior of operator matrix elements and the spectral properties of the Hamiltonian, it is more convenient to rewrite it as a functional of the density matrix $\rho(x, x')$. The first step is to consider the Fourier transform $G_t(\mu, \mu)$ of the tomographic density $M_t(X, \mu, \nu)$

$$G_t(\mu, \nu) \doteq G_t(1, \mu, \nu) = \int d^n X\, e^{iX \bullet \mathbf{1}} M_t(X, \mu, \nu) \tag{7}$$

and perform the integrals in (1) to obtain

$$\lambda_{\binom{v_1}{v_2}} = \lim_{t \to \infty} \frac{1}{t} \log \left\| \begin{matrix} \nabla_\mu G_t(\mu, \nu)\,|_{\mu=\nu=0} \\ \nabla_\nu G_t(\mu, \nu)\,|_{\mu=\nu=0} \end{matrix} \right\|. \tag{8}$$

Now, using the relation between the tomographic densities and the density matrix [2], namely,

$$G_t(\mu, \nu) = \left(\frac{1}{2\pi}\right)^n \int d^n X\, d^n p\, d^n x\, d^n x'\, e^{i(X \bullet \mathbf{1} - p \bullet (x - x'))} \rho_t(x, x') \delta^n\left(X - \mu \circledast \left(\tfrac{x+x'}{2}\right) + \upsilon \circledast p\right) \tag{9}$$

one easily obtains

$$\lambda_{\binom{v_1}{v_2}} = \lim_{t \to \infty} \frac{1}{t} \log \left\| \begin{matrix} \mathrm{Tr}\{\rho_t x\} \\ \mathrm{Tr}\{\rho_t p\} \end{matrix} \right\| \tag{10}$$

the density matrix at time zero (corresponding to $M_0(X', \mu', \nu')$ in Eq. (3)) being

$$\rho_0(x, x') = -e^{ip_0 \bullet (x - x')} \left\{ (v_1 \bullet \nabla) \delta^n\left(q_0 - \tfrac{x+x'}{2}\right) + i v_2 \bullet (x - x') \delta^n\left(q_0 - \tfrac{x+x'}{2}\right) \right\}. \tag{11}$$

Eq. (10) means that the quantum Lyapunov exponent measures the exponential rate of growth of the expectation values of position and momentum, starting from the initial singular perturbation ρ_0. This is a rather appealing and intuitive form for the Lyapunov exponent. That the quantum Lyapunov exponent should have a form of this type had already been proposed in Ref. [6], based on qualitative physical considerations. What is not obvious, though, without the tomographic formulation, is that this is the form that corresponds exactly to the same physical quantity as the classical Lyapunov exponent. Also non-obvious is the specific form that the initial singular perturbation ρ_0 should take.

Using the time-dependent operators in the Heisenberg picture

$$x_H(t) = U^\dagger x U, \qquad p_H(t) = U^\dagger p U, \tag{12}$$

one has an equivalent form for $\lambda_{\vec{v}}$

$$\lambda_{\binom{v_1}{v_2}} = \lim_{t \to \infty} \frac{1}{t} \log \left\| \begin{matrix} \mathrm{Tr}'\{\rho_0 x_H(t)\} \\ \mathrm{Tr}'\{\rho_0 p_H(t)\} \end{matrix} \right\|, \tag{13}$$

where we have also defined

$$\mathrm{Tr}'\{\rho_0 x_H(t)\} = \mathrm{Tr}\{\rho_0 x_H(t)\} / \mathrm{Tr}\{\rho_0 x_H(0)\}.$$

Whenever $\rho_0 x_H(t)$ is a trace class operator, the term corresponding to $\mathrm{Tr}\{\rho_0 x_H(0)\}$ has no contribution in the $t \to \infty$ limit. On the other hand, by taking the appropriate cut-off and a limiting procedure, the above expression may also make mathematical sense even in some non-trace class cases.

3. An example: kicked motions in the torus

Let $x_1, x_2 \in [-\pi, \pi)$ be coordinates in the 2-torus T^2 with conjugate momenta p_1, p_2 and the dynamics be defined by the Hamiltonian

$$H = H_0 + \sum_n V(x, p)\delta(t - n\tau) \tag{14}$$

$x \in T^2$, $p \in R^2$ and, in particular, $H_0 = p^2/2$. Let

$$\mathcal{H} = \mathcal{L}^2\big([-\pi, \pi), d^2x\big). \tag{15}$$

Physical observables should be self-adjoint operators. Therefore the domain $D(x_i)$ of x_i is

$$D(x_i) = \{f \in \mathcal{H}\} \tag{16}$$

and the domain of p_i

$$D(p_i) = \big\{f \in \mathcal{H} \;\big|\; f(x_i = -\pi) = f(x_i = \pi)\big\}. \tag{17}$$

A convenient basis of vectors in $D(p_i)$ is

$$\mathcal{H} = \left\{ \langle x|q\rangle = \frac{1}{\sqrt{2\pi}} e^{iq\bullet x} \;\middle|\; k \in Z^2 \right\}. \tag{18}$$

The Floquet operator associated to the periodic Hamiltonian H is

$$U_F = U_0 U_K \tag{19}$$

with $U_0 = \exp(iH_0\tau)$ and

$$U_K = \exp(iV(x, p)). \tag{20}$$

We will consider different types of kick potentials. Whenever $V(x, p)$ is a function of x or p alone, any differentiable function will generate an unitary operator U_K operating in the basis (18). However, for kicks of the electromagnetic type, $V(x, p) = \frac{1}{2}(x_i p_i + p_i x_i)$, because

$$D\big(\tfrac{1}{2}(x_i p_i + p_i x_i)\big) = D(x_i p_i) \cap D(p_i x_i) = \{f \in \mathcal{H} \mid f(x_i = -\pi) = -f(x_i = \pi)\}. \tag{21}$$

$\frac{1}{2}(x_i p_i + p_i x_i)$ does not generate a continuous unitary group in (18) and only a discrete set of kicks will be acceptable, namely,

$$U_K = \exp\big(\tfrac{1}{2}(x \bullet A \bullet p + p \bullet A \bullet x)\big) \tag{22}$$

$\exp(A)$ being a 2×2 matrix with integers entries and determinant one, the last condition resulting from

$$e^{\frac{1}{2}(x\bullet A\bullet p + p\bullet A\bullet x)} = e^{x\bullet A\bullet p} e^{\frac{1}{2}\operatorname{Tr} A}.$$

Using the momentum basis (18) the initial density matrix ρ_0 of Eq. (11) may be written

$$\rho_0 = -2\left(v_1 \bullet \frac{\partial}{\partial q_0} + v_2 \bullet \frac{\partial}{\partial p_0}\right) \sum_{k \in Z^2} |p_0 - k\rangle e^{i2k \bullet q_0} \langle p_0 + k| \tag{23}$$

and in a position (generalized) eigenstate basis

$$\rho_0 = -4\pi \left(v_1 \bullet \frac{\partial}{\partial q_0} + v_2 \bullet \frac{\partial}{\partial p_0}\right) \int_{T^2} d^2x \, |q_0 + x\rangle e^{i2x \bullet p_0} \langle q_0 - x|. \tag{24}$$

The corresponding traces, needed to compute the Lyapunov exponent, are

$$\mathrm{Tr}\left\{\rho_0 U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t \right\} = -2\left(v_1 \bullet \frac{\partial}{\partial q_0} + v_2 \bullet \frac{\partial}{\partial p_0}\right) \sum_{k \in Z^2} e^{i2k \bullet q_0} \langle p_0 + k| U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t |p_0 - k\rangle \tag{25}$$

and

$$\mathrm{Tr}\left\{\rho_0 U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t \right\} = -4\pi \left(v_1 \bullet \frac{\partial}{\partial q_0} + v_2 \bullet \frac{\partial}{\partial p_0}\right) \int_{T^2} d^2x \, e^{i2x \bullet p_0} \langle q_0 - k| U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t |q_0 + x\rangle. \tag{26}$$

Another form, that will be used later on, is a spectral decomposition using the eigenmodes of the Floquet operator. For discrete spectrum

$$\mathrm{Tr}\left\{\rho_0 U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t \right\} = \sum_{\mu,\nu} \langle E_\mu|\rho_0|E_\nu\rangle \langle E_\nu| \begin{pmatrix} x \\ p \end{pmatrix} |E_\mu\rangle e^{-i(E_\mu - E_\nu)t} \tag{27}$$

and in general

$$\mathrm{Tr}\left\{\rho_0 U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t \right\} = \int dE_\mu \, dE_\nu \, \rho_0(\mu,\nu) \begin{pmatrix} x(\nu,\mu) \\ p(\nu,\mu) \end{pmatrix} e^{-i(E_\mu - E_\nu)t}. \tag{28}$$

Three types of potentials will be considered.

Case 1. $V(x, p) = 0$.

This is just free motion on the torus with $U_t = \exp\left(i \frac{p^2}{2} t\right)$. Then

$$U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t = \begin{pmatrix} x + tp \\ p \end{pmatrix}$$

and from (25) it follows that $\mathrm{Tr}\left\{\rho_0 U_t^\dagger \binom{x}{p} U_t\right\}$ is a constant independent of time, implying $\lambda_v = 0$. A similar conclusion would be obtained analyzing the spectral decomposition because the spectrum of the Floquet being discrete in this case the right-hand-side of Eq. (27) is an almost periodic function.

Free motion having an irrelevant effect on the computation of the Lyapunov exponent, we restrict ourselves, for simplicity, to the resonant case, $\tau = 4\pi m$, $m \in Z$, in the next two examples.

Case 2. $V(x, p) = \alpha \mathrm{g}(x)$ and $\tau = 4\pi m$, $m \in Z$.

From

$$\langle p_0 + k| U_t^\dagger \begin{pmatrix} x \\ p \end{pmatrix} U_t |p_0 - k\rangle = \langle p_0 + k| \begin{pmatrix} x \\ p + \frac{t}{\tau}\alpha \nabla g(x) \end{pmatrix} |p_0 - k\rangle$$

it follows that $\mathrm{Tr}\left\{\rho_0 U_t^\dagger \binom{x}{p} U_t\right\}$ grows at most linearly with t, implying also $\lambda_v = 0$.

In this case the Floquet operator spectrum is continuous but the kernels $x(\nu,\mu)$ and $p(\nu,\mu)$ being

$$x(\nu,\mu) \sim \delta(E_\nu - E_\mu), \qquad p(\nu,\mu) \sim \delta'(E_\nu - E_\mu),$$

we obtain the same conclusion from the spectral representation (28).

Case 3. $V(x,p) = \frac{1}{2}(x \bullet A \bullet p + p \bullet A \bullet x)$, $\tau = 4\pi m$, $m \in Z$ and $M = \exp(A) = \left(\begin{smallmatrix} 1 & 1 \\ 1 & 2 \end{smallmatrix}\right)$.

Let $t = n\tau$. From

$$\langle p_0 + k | U_t^\dagger x U_t | p_0 - k \rangle = \left((M^{-1})^T\right)^n \langle p_0 + k | x | p_0 - k \rangle$$

and

$$\langle p_0 + k | U_t^\dagger p U_t | p_0 - k \rangle = M^n \langle p_0 + k | p | p_0 - k \rangle$$

with

$$M^n = \begin{pmatrix} \omega^{-2n+1} + \omega^{2n-1} & -\omega^{-2n} + \omega^{2n} \\ -\omega^{-2n} + \omega^{2n} & \omega^{-2n-1} + \omega^{2n+1} \end{pmatrix}, \qquad M^{-n} = \begin{pmatrix} \omega^{2n+1} + \omega^{-2n-1} & -\omega^{2n} + \omega^{-2n} \\ -\omega^{2n} + \omega^{-2n} & \omega^{2n-1} + \omega^{-2n+1} \end{pmatrix}$$

and $\omega = \frac{1}{2}(1 + \sqrt{5})$, we conclude working out Eq. (25) that in this case there is a non-zero Lyapunov exponent $\lambda_v = 2 \log \omega$.

It is instructive to find out how the same result may be obtained from the spectral representation (28). In the resonant case ($\tau = 4\pi m$) the eigenstates of the Floquet operator are [7]

$$|E_\alpha\rangle = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} e^{-i\alpha n} \left| M^n P \right\rangle$$

with eigenvalue $\exp(-i\alpha)$. From

$$\langle E_\mu | U_t^\dagger p U_t | E_\alpha \rangle = M^n \langle E_\mu | p | E_\alpha \rangle = e^{-i(E_\alpha - E_\mu) n\tau} \langle E_\mu | p | E_\alpha \rangle,$$

and the corresponding equation for x, it follows that the kernels $x(\nu,\mu)$ and $p(\nu,\mu)$ are linear combinations of

$$\delta\left(E_\alpha - E_\mu - \tfrac{i}{\tau} \log \lambda_k\right),$$

λ_k, $k = 1, 2$, being the eigenvalues of the matrix M. It is the complex shift in the argument of the delta that converts the complex exponentials in the spectral decomposition (28) into an exponential growing quantity.

In both Cases 2 and 3 the Floquet spectrum is absolutely continuous. Nevertheless the rate of growth of the traces is quite different. These examples suggest that the critical role is actually played by the analytic nature of the phase-space operator kernels $x(\nu,\mu)$ and $p(\nu,\mu)$. This will further clarified in Section 4.

4. Sensitive dependence in quantum mechanics [8,9]

Let us denote the dynamical variable appearing in Eq. (13) as

$$\Delta(t) = \left\| \begin{matrix} \mathrm{Tr}'\{\rho_0 x_H(t)\} \\ \mathrm{Tr}'\{\rho_0 p_H(t)\} \end{matrix} \right\|. \tag{29}$$

In the three examples studied in the preceding section this dynamical quantity shows no growth in the free motion case, polynomial growth for space-dependent kicks and exponential growth for the electromagnetic-like kicks. The second case, as well as the study of the standard map in Ref. [2], clearly show the taming effect that quantum mechanics has on classical chaos. Nevertheless $\Delta(t)$, as defined in Eq. (29), is the quantum observable that corresponds to the notion of separation of nearby trajectories in the classical case. Therefore, for example, a polynomial growth of this observable signals an higher degree of dynamical complexity that no growth at all. Therefore, in view of the widespread quantum suppression of exponential growth, it makes sense to characterize different degrees of quantum dynamical complexity by a more general notion of sensitive dependence. We define:

Definition. Quantum dynamics is sensitive-dependent in the support of ρ_0 if for any T and $M > 0$, there is a $t > T$ such that $(\Delta(t)/\Delta(0)) > M$.

The above definition allows for rates of growth slower than exponential and even for oscillations of the ratio $\Delta(t)/\Delta(0)$. It only requires it to be unbounded.

In the examples of the preceding section, free motion is not sensitive-dependent, whereas the x-dependent kicks in Case 2 are polynomial sensitive-dependent and the non-local (electromagnetic) kicks in Case 3 in Section 3 are exponential sensitive-dependent.

A precise mathematical characterization of when each type of sensitive-dependence is to be expected, is possible. This uses the well-known space of ultradistributions of compact support [4,5] and the corresponding Fourier image.

Let $X_n = \{z : z \in \mathbb{C},\ |z| > n\}$ and $\mathcal{B}_n$ be the Banach space of complex functions analytic in X_n and continuous in $\overline{X_n}$ with norm

$$\|\phi\|_n = \sup_{z \in X_n} |\phi(z)|. \tag{30}$$

The space of ultradistributions of compact support $\mathcal{U}_c$ is the inductive limit of the spaces $\mathcal{B}_n$. Its dual is the space of entire functions. An important subspace of $\mathcal{U}_c$ is the space of distributions of compact support $\mathcal{D}_c$, the correspondence being established by the injective (but not surjective) mapping (the Stieltjes transform)

$$Sf(z) = \frac{1}{2\pi i} \int_\Gamma \frac{f(\lambda)}{\lambda - z}\, d\lambda. \tag{31}$$

Whenever f is a distribution of compact support, the ultradistribution $Sf \in \mathcal{U}_c$ vanishes at infinity.

On the other hand the Fourier transform establishes a correspondence between the space of ultradistributions of compact support and the space of functions of exponential growth.

An entire function $\Psi(z)$ is said to be of exponential growth if and only if there are constants α and β such that $|\Psi(z)| \leqslant \alpha e^{\beta|z|}$, $\forall z \in \mathbb{C}$. The vector space of these functions will be denoted by $\mathcal{H}_e$. The Fourier transform

$$(\mathcal{F}\phi)(x) = \int_\Gamma e^{ix\lambda} \phi(\lambda)\, d\lambda \tag{32}$$

with $\phi \in \mathcal{U}_c$ is a bijective linear map of $\mathcal{U}_c$ over $\mathcal{H}_e$.

On the other hand the restriction of $\mathcal{F}$ to the subspace $\mathcal{D}_c$ establishes an isomorphism between $\mathcal{D}_c$ and the subspace of $\mathcal{H}_e$ consisting of entire functions with polynomially bounded growth on horizontal strips around the real axis.

Now noticing that, in the energy differences $(E_\mu - E_\nu)$ variable, the integral in Eq. (28) is the Fourier transform of the kernels

$$\mathcal{K}(\mu, \nu) = \rho_0(\mu, \nu) \begin{pmatrix} x(\nu, \mu) \\ p(\nu, \mu) \end{pmatrix} \tag{33}$$

we conclude:

Proposition. *A necessary condition for exponential sensitive dependence in quantum dynamics is that the kernel $\mathcal{K}(\mu, \nu)$ as a function of the energy differences $E_\mu - E_\nu$ be a member of $\mathcal{U}_c/\mathcal{D}_c$. If the kernel belongs to $\mathcal{D}_c$ then there is, at most, polynomial growth.*

Cases 2 and 3 in Section 3 are examples where the kernels belong in the first case to $\mathcal{D}_c$ and in the second to $\mathcal{U}_c/\mathcal{D}_c$.

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