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ON THE NOTION OF QUANTUM LYAPUNOV EXPONENT

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Abstract. Classical chaos refers to the property of trajectories to diverge exponentially as time $t \to \infty$. It is characterized by a positive Lyapunov exponent. There are many different descriptions of quantum chaos. One description related to the notion of generalized (quantum) Lyapunov exponent is based either on qualitative physical considerations or on the so-called symplectic tomography map. The purpose of this paper is to show how the definition of quantum Lyapunov exponent naturally arises in the framework of the Moyal phase-space formulation of quantum mechanics and is based on the notions of quantum trajectories and the family of quantizers. The role of the Heisenberg uncertainty principle in the statement of the criteria for quantum chaos is made explicit.

1. Introduction

The irregular behavior of classical dynamical systems arising from deterministic time evolution without any external randomness and stochasticity—the so-called deterministic chaos—manifests itself as an extremely sensitive dependence on the initial conditions, which makes unstable the long-term prediction of the dynamics. In such a system, a positive Lyapunov exponent is a quantitative measure of the infinite-time exponential separation of neighboring orbits.

In detail, let a system have the form $\dot{x} = F(x)$, where $x = (q, p)$ is a d-dimensional vector from the phase space of the system. Denote by $x(t, x_0)$ its solution with initial point at x_0 and $t \in (0, \infty)$. Then the Lyapunov exponent is given by

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln \frac{\|\delta x(t)\|}{\|\delta x(0)\|}.$$

Here $\|\cdot\|$ represents the d-dimensional Euclidean norm, and $\|\delta x(0)\|$ is an initial infinitesimal deviation from x_0 and $\|\delta x(t)\| = \big\|x\big(t, x_0 + \delta x(0)\big) - x(t, x_0)\big\|$ is the deviation from $x(t, x_0)$ at time t. In the limit as $\|\delta x(0)\| \to 0$, one obtains

$$\lambda_v = \lim_{t\to\infty} \frac{1}{t} \ln \|(v \cdot \nabla_{x_0}) x(t, x_0)\|, \tag{1}$$

where $v \in \mathbb{R}^d$ is a unit vector in the direction of the initial displacement $\delta x(0)$ and ∇_{x_0} is the gradient with respect to the initial point x_0.

To extend this notion to quantum mechanics, it is natural to use its phase-space formulation where quantum observables on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n, \mathbb{C})$ are represented by functions on the phase space called symbols. Consider the Weyl symbol $A(x)$ obtained from the operator $\hat{A}$ such that

$$\hat{A}\psi(q') \equiv \int \langle q'|\hat{A}|q''\rangle\langle q''|\psi\rangle\, dq'', \quad \psi \in \mathcal{H},$$

by the formula

$$A(x) = 2^n \int e^{2ips/\hbar} \langle q - s|\hat{A}|q + s\rangle\, ds \equiv [\hat{A}]_{\mathrm{w}}(x). \tag{2}$$

The dimension of the phase space is even, $d = 2n$.

In this case, the quantum mechanical mean value

$$\langle \hat{A}\rangle_\rho = \mathrm{Tr}\, \hat{A}\hat{\rho} = \int \langle q'|\hat{A}|q''\rangle\langle q''|\hat{\rho}|q'\rangle\, dq'\, dq'' \tag{3}$$

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can be written in a form analogous to classical statistical mechanics:

$$\langle \hat{A} \rangle_\rho = \int A(x) W(x)\, dx, \tag{4}$$

which gives the mean value of A in the state $\rho(x) = [\hat{\rho}]_{\rm w}(x)$. Here W is the Wigner distribution function $W(x) = h^{-n}\rho(x)$.

One drawback of this approach, relative to the classical statistical density, is that the $W(x)$ is not everywhere nonnegative and so is not a conventional probability density.

To circumvent this difficulty, another representation can be considered in which a new density is defined as the Radon transform [3] of the Wigner function $W(x)$. It takes only nonnegative values and becomes a straightforward analog of the classical statistical density. In [2], it was shown that the tomographic representation of quantum mechanics based on the Radon transform is an alternative to the Weyl–Wigner formalism.

Due to their similar nature in the quantum and classical cases, the tomographic distributions were used in [7] to define a quantum Lyapunov exponent. In detail, let $U(t) = \exp[-it\hat{H}/\hbar]$ be the Schrödinger unitary evolution operator and $\hat{X}(t) = U^{+}(t)\hat{x}U(t)$ be time evolution of the quantum coordinate operators $\hat{x} = (\hat{p}, \hat{q})$. The formula for a quantum Lyapunov exponent turned out to be

$$\Lambda_v = \lim_{t\to\infty} \frac{1}{t} \ln \|\langle \hat{X}(t) \rangle_{\rho_0^v}\|, \tag{5}$$

where the average is taken with respect to a special initial singular density $\hat{\rho}_0^v$, the kernel of which has the form

$$\langle q'|\hat{\rho}_0^v|q''\rangle = e^{ip_0(q'-q'')/\hbar} \left((v_1\nabla) + \frac{iv_2(q'-q'')}{\hbar} \right) \delta\left(q_0 - \frac{q'+q''}{2} \right). \tag{6}$$

Here parameters (q_0, p_0) correspond to the initial point x_0 in the phase space and the vector $v = (v_1, v_2) \in \mathbb{R}^d$ defines the direction of the initial deviation from x_0. Man'ko and Vilela Mendes [7] stress the special role of the tomographic distributions in obtaining these formulas, in particular, the formula for the initial density (6). In [11], a similar formula is obtained from qualitative considerations, but the choice of the initial density appears rather *ad hoc* in the quantum mechanical setting. As is shown in [7,11], the quantum Lyapunov exponent (5), (6) helps to classify different types of quantum complexity. There are examples where an exponential rate of growth for the trace $\langle \hat{X}(t) \rangle_{\rho_0^v} = \operatorname{Tr} \hat{X}(t)\hat{\rho}_0^v$ of position and momentum observables starting from the singular initial density matrix (6) was found in quantum mechanics. In many cases where quantum mechanics has a damping effect on the classical chaos and the rate of growth for the trace is milder than exponential, the notion of quantum sensitive dependence was used instead.

In this paper, we derive representations of the quantum Lyapunov index from the Weyl–Stratonovich quantizer [10]. Using the notion of quantum trajectory [8], i.e., the symbol of the operator $\hat{X}(t)$, we rewrite the formula for the quantum Lyapunov exponent in a form identical to the classical definition (1) (see formula (22)), replacing the classical trajectory $x(t, x_0)$ with the quantum trajectory $X(x_0, t; \hbar)$. In this form, it becomes transparent that the definition respects the correspondence principle: in the limit as $\hbar \to 0$, the definition of the quantum Lyapunov exponent transforms into the classical definition. In contrast to the classical trajectory, the Heisenberg uncertainty principle prevents the quantum trajectory from being interpreted as a measurable physical value, despite the fact that it can be viewed as the limit of a sequence of quantum means.

2. Quantum Phase Space. Weyl–Stratonovich Quantizer

The development of the phase-space formulation of quantum mechanics has a long history, but it still is of interest due to the extensive study of possible generalizations to the case of non-Abelian gauge theory with support on a Riemannian manifold.

In 1932, Wigner introduced his quasi-probability distribution associated with the wave function $\psi(q)$:

$$W(x) = \left(\frac{2}{h}\right)^n \int e^{2ips/\hbar}\psi^+(q-s)\psi(q+s)\,ds, \quad h = 2\pi\hbar. \tag{7}$$

Further developing Groenewold's ideas published in 1946, Moyal, in his paper of 1949, gave a statistical interpretation of Wigner's formula as a Fourier inverse of the expectation value of the Heisenberg translation operator

$$T(y) \equiv e^{-2iJy\cdot\hat{x}/\hbar}, \quad T(x)^+\hat{x}T(x) = \hat{x} - 2xI, \tag{8}$$

namely,

$$W(x) = \left(\frac{2}{h}\right)^{2n} \int e^{2ix\cdot Jy/\hbar}\langle\psi|T(y)|\psi\rangle\,dy,$$

where J denotes the Poisson matrix

$$\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

He also showed that the Wigner rule (7) of getting the phase-space function from the operator $|\psi\rangle\langle\psi|$ (and $\hat{A}$) is inverse to the Weyl quantization rule:

$$\langle q'|\hat{A}|q''\rangle = h^{-n}\int e^{ip(q'-q'')/\hbar}A\left(\frac{q'+q''}{2}, p\right)\,dp. \tag{9}$$

A significant step further was the introduction [5,9,10] of the family of unitary operators $\Delta(x)$ labeled by points of the phase space. These operators define both quantization (9) and dequantization (2) rules, which establish a unitary isomorphism between symbols and operators:

$$A(x) = 2^n\,\mathrm{Tr}\,\Delta(x)\hat{A}, \quad \hat{A} = \int A(x)\Delta(x)\,d^*x. \tag{10}$$

For this reason, the operators $\Delta(x)$ are called quantizers. Above, $d^*x = (\pi\hbar)^{-n}\,dx$ denotes a dimensionless phase-space measure.

The fundamental nature of quantizers also reveals itself in the fact that they define the noncommutative product $*$ for the phase-space functions

$$(A*B)(x) = \int A(y)B(z)K(x,y,z)\,dy\,dz, \quad K(x,y,z) = \frac{2^n}{(\pi\hbar)^{2n}}\,\mathrm{Tr}\,\Delta(x)\Delta(y)\Delta(z).$$

Other useful properties [6] of quantizers are as follows:

(1) $\Delta(x) = \Delta(x)^+ = \Delta(x)^{-1}$. Thus, $\Delta(x)^2 = I$ and $\|\Delta(x)\| = 1$;
(2) $\mathrm{Tr}\,\Delta(x) = 2^{-n}$;
(3) $\mathrm{Tr}[\Delta(x)\Delta(x')] = (\pi\hbar/2)^n\delta(x-x')$;
(4) $\Delta(x) = \int e^{2ix\cdot Jy/\hbar}T(y)d^*y$;
(5) $\rho(x) = 2^n\langle\psi|\Delta(x)|\psi\rangle$;
(6) $\Delta(0)\hat{x}\Delta(0) = -\hat{x}$;
(7) $\Delta(x) = T(x/2)^+\Delta(0)T(x/2)$;
(8) $\int \Delta(x)d^*x = I$.

Many authors (see, e.g., [4]) used quantizers as a fundamental object defining the deformation quantization introduced in 1978 in [1].

There is one observation useful for the purpose of our note. In view of the first equation of (10), property (3) shows that the symbol of the quantizer is $[\Delta(x)]_{\mathrm{w}}(x') = (h/2)^n\delta(x-x')$, and by (9) that its kernel is

$$\langle q'|\Delta(x)|q''\rangle = 2^{-n}e^{ip(q'-q'')/\hbar}\delta\left(q - \frac{q'+q''}{2}\right). \tag{11}$$

An attractive feature of the quantum phase space is computation of the trace of an operator and pairs of operators. For operators $\hat{A}$ and $\hat{B}$ with symbols $A(x)$ and $B(x)$, one has

$$\operatorname{Tr}\hat{A} = \frac{1}{h^n}\int A(x)\,dx, \tag{12}$$

$$\operatorname{Tr}\hat{A}\hat{B} = \frac{1}{h^n}\int A * B(x)\,dx = \frac{1}{h^n}\int A(x)B(x)\,dx. \tag{13}$$

Identity (12) follows from (10) and property (2). The removal of the operation $*$ in (13) is a consequence of properties (3) and (8).

3. Quantum Means and Symbols

The mean value of a quantum observable given by an operator $\hat{A}$ in a unit normalized quantum state $\psi(q)$ is

$$\langle\psi|\hat{A}|\psi\rangle = \operatorname{Tr}\hat{A}\hat{\rho}, \quad \hat{\rho} = |\psi\rangle\langle\psi|. \tag{14}$$

This is an example of formula (3) for the pure state density. Its phase-space form is (4), which is a special case of the trace identity (13).

Let us consider a family of Gaussian states localized near $q = q_0 \in \mathbb{R}^n$ with width $\sqrt{\hbar}$:

$$\psi_\hbar(q; q_0, p_0) = \frac{1}{(\pi\hbar)^{n/4}}\exp\left(-\frac{(q-q_0)^2}{2\hbar} + \frac{i}{\hbar}p_0(q-q_0)\right).$$

These states are all unit normalized, $\|\psi_\hbar(q_0, p_0)\| = 1$. By formula (7), the corresponding normalized Wigner function has the form

$$W_\hbar(x; q_0, p_0) = \frac{1}{(\pi\hbar)^n}\exp\left(-\frac{(q-q_0)^2 + (p-p_0)^2}{\hbar}\right).$$

We make the following two important remarks about this function.

Remark 1. The function $W_\hbar(x; x_0)$ is positive and thus can be interpreted as the classical statistical density.

Remark 2. In view of the formula

$$\lim_{\hbar\to 0} W_\hbar(x; x_0) = \delta(x - x_0), \tag{15}$$

it is obvious that the symbol of the quantizer $\Delta(x)$ is proportional to the limit of the sequence of Wigner functions $W_\hbar(x; x_0)$ of the localized Gaussian states as their width $\sqrt{\hbar}$ tends to 0.

Thus, the $\hbar$-independent symbol $A(x_0)$ of an operator $\hat{A}$ evaluated at a point x_0 of the phase space appears as the mean value calculated with respect to the localized Gaussian state with parameters $x_0 = (q_0, p_0)$ in the limit as the width of the state tends to zero:

$$\lim_{\hbar\to 0}\langle\psi_\hbar(q; x_0)|\hat{A}|\psi_\hbar(q; x_0)\rangle = \lim_{\hbar\to 0}\int A(x)W_\hbar(x; x_0)\,dx = A(x_0).$$

Note that this limit process takes one outside the framework of quantum expectation values. The norm $\|\Delta(x)\| = 1$ implies that for any pure state $\hat{\rho} = |\psi\rangle\langle\psi|$

$$|\rho(x)| \le 2^n, \quad |W(x)| \le \left(\frac{2}{h}\right)^n. \tag{16}$$

This means that the quantizer or any singular symbol such as $\delta(x - x_0)$ does not correspond to a pure state. The global bound (16) forces $\rho(x)$ to be distributed in the phase space without large peaks and is an obvious consequence of the uncertainty principle.

Let a quantum operator $\hat{A}$ have a Weyl symbol $A(x)$ and the time-dependent operator $\hat{A}(t) = U^{+}(t)\hat{A}U(t) = A\big(\hat{X}(t)\big)$ have the Weyl symbol $A(x,t;\hbar)$ such that $A(x,0;0) = A(x)$. Now consider the expression

$$\langle A\rangle(t,x_0;\hbar,\varepsilon) = \int W_\varepsilon(x;x_0)A(x,t;\hbar)\,dx$$

as a function of two small parameters $\hbar$ and ε. The following table shows the meaning of the expression if one or both of the parameters are 0.

$\langle A\rangle(t,x_0;\hbar,\varepsilon)$	$\hbar \to 0$	$\hbar \neq 0$
$\varepsilon \to 0$	classical observable $A\big(x(t,x_0)\big)$	symbol $A(x_0,t;\hbar)$ of quantum observable $\hat{A}(t)$
$\varepsilon \neq 0$	classical statistical mean $\int dy W_\varepsilon(y;x_0)A\big(x(t,y)\big)$	quantum mechanical mean value

Note that the function W_ε for $\varepsilon \neq \hbar$ does not correspond to a pure state $\psi(q)$ but rather is a density matrix.

4. Classical and Quantum Lyapunov Exponents

From the table, we see that the symbol $A(x_0,t;\hbar)$ is, in fact, a quantum analog of the classical value $A\big(x(t,x_0)\big)$. This is due to the Egorov theorem, which states that

$$\lim_{\hbar\to 0} A(x,t;\hbar) = A\big(x(t,x_0)\big), \tag{17}$$

where $x(t,x_0)$ is a classical trajectory.

Thus, the quantum analog of $(v\cdot\nabla_{x_0})A\big(x(t,x_0)\big)$ is $(v\cdot\nabla_{x_0})A(x_0,t;\hbar)$.

From the first formula of (10) one has

$$A(x_0,t;\hbar) = 2^n \int \langle q'|\Delta(x_0)|q''\rangle\langle q''|\hat{A}(t)|q'\rangle\,dq''\,dq'.$$

Here we see that the complete information about the point x_0 of the phase space is contained in the quantizer kernel $\langle q'|\Delta(x_0)|q''\rangle$. Thus, the derivative $(v\cdot\nabla_{x_0})$ will only affect this part of the formula:

$$(v\cdot\nabla_{x_0})A(x_0,t;\hbar) = 2^n \int [(v\cdot\nabla_{x_0})\langle q'|\Delta(x_0)|q''\rangle]\langle q''|\hat{A}(t)|q'\rangle\,dq''\,dq'.$$

From (11) we obtain

$$2^n(v\cdot\nabla_{x_0})\langle q'|\Delta(x_0)|q''\rangle = \langle q'|\hat{\rho}_0^v|q''\rangle,$$

where $\langle q'|\hat{\rho}_0^v|q''\rangle$ is given by (6). Therefore, we have

$$(v\cdot\nabla_{x_0})A(x_0,t;\hbar) = \int \langle q'|\hat{\rho}_0^v|q''\rangle\langle q''|\hat{A}(t)|q'\rangle\,dq''\,dq' = \langle\hat{A}(t)\rangle_{\rho_0^v}. \tag{18}$$

Now let $A(x)$ be a vector function. Introduce the notation

$$\Lambda_v^A(x_0;\hbar) = \lim_{t\to\infty}\frac{1}{t}\ln\|(v\cdot\nabla_{x_0})A(x_0,t;\hbar)\|. \tag{19}$$

Using (18), we can also write

$$\Lambda_v^A(x_0;\hbar) = \lim_{t\to\infty}\frac{1}{t}\ln\|\langle\hat{A}(t)\rangle_{\rho_0^v}\|. \tag{20}$$

Taking limit $\hbar\to 0$ in (19), we obtain

$$\Lambda_v^A(x_0;0) = \lim_{t\to\infty}\frac{1}{t}\ln\big\|(v\cdot\nabla_{x_0})A\big(x(t,x_0)\big)\big\|. \tag{21}$$

This formula is well defined for a class of vector functions $A(x)$. To obtain the classical Lyapunov exponent, one must make, however, the special choice $A(x) = x$. Then formula (21) becomes exactly (1).

In the quantum case, the symbol $A(x) = x$ defines an operator $\hat{x}$ which makes it possible to talk about the *quantum trajectory* [8] defined as the symbol of $\hat{X}(t) = U^+(t)\hat{x}U(t)$:

$$X(x_0, t; \hbar) = \lim_{\varepsilon\to 0} \operatorname{Tr} \hat{X}(t)\hat{\rho}_\varepsilon = \lim_{\varepsilon\to 0} \int X(x, t; \hbar) W_\varepsilon(x; x_0)\, dx.$$

Then formula (20) gives us the definition of the quantum Lyapunov exponent, which coincides with (5) and (6).

In view of (17), $\lim_{\hbar\to 0} X(x_0, t; \hbar) = x(t, x_0)$, and the notion of quantum trajectory and (19) and (20) allows us also to write (5) in a form similar to (1):

$$\Lambda_v = \Lambda_v^X(x_0; \hbar) = \lim_{t\to\infty} \frac{1}{t} \ln\{(v \cdot \nabla_{x_0}) X(x_0, t; \hbar)\}. \tag{22}$$

5. Radon Transform and Tomographic Procedure

We make a few comments on the approach presented in [7]. To simplify the exposition of some formulas and their geometrical meaning, we assume in this section that $n = 1$, i.e., $q \in \mathbb{R}^1$, and $x \in \mathbb{R}^2$.

Although the integral of the Wigner function for the density matrix $|\psi\rangle\langle\psi|$ is always 1, typically there are regions in the phase space where $W(x)$ is negative. This behavior results from the spectral expansion of the quantizer. Property (1) shows that the spectrum of $\Delta(x)$ is ± 1 for all x. In detail,

$$\Delta(x) = P_+(x) - P_-(x), \quad I = P_+(x) + P_-(x), \tag{23}$$

where $P_\pm(x)$ are the spectral projectors for the eigenvalues ± 1. If $x = 0$, then $\Delta(0)$ is the parity operator on $\mathcal{H}$ and $P_\pm(0)$ are the corresponding even and odd projectors. If $x \neq 0$, then $P_\pm(x)$ are the Heisenberg translates of these operators, namely $T(x/2)^+ P_\pm(0) T(x/2)$. Applying (23) to $W(x)$, we obtain the Royer expansion $W(x) = \frac{2}{\hbar}\bigl[\|P_+(x)\psi\|^2 - \|P_-(x)\psi\|^2\bigr]$. Therefore, whenever $\|P_+(x)\psi\| < \|P_-(x)\psi\|$, $W(x)$ is negative. This makes it impossible to interpret it as a classical statistical density.

Nevertheless, the two physically important *projections* of the $W(x)$, namely,

$$\int W(q, p)\, dp = |\psi(q)|^2, \quad \int W(q, p)\, dq = |\tilde{\psi}(p)|^2,$$

are positive and form corresponding marginal distributions. Here $\tilde{\psi}(p) = h^{-n/2} \int \psi(q) e^{-ipq/\hbar}\, dq$ is the wave function in the momentum representation.

One may consider a family of *projections* with respect to all directions in the phase space, not only the two given above. In this way, we obtain the Radon transform of $W(x)$

$$RW(Q, \xi, \eta) = \int W(q, p) \delta(Q - q\xi - p\eta)\, dq\, dp.$$

Here $Q - q\xi - p\eta = 0$ is the equation of a line in the phase space. Rewriting the above formula as

$$RW(Q, \xi, \eta) = \frac{1}{2\pi} \int W(q, p) e^{-ik(Q - q\xi - p\eta)}\, dk\, dq\, dp = \frac{1}{2\pi} \int dk e^{-ikQ} \int dq\, dp\, W(q, p) e^{i(kq\xi + kp\eta)},$$

one can see two remarkable features. First, the right-hand side can be viewed as the inverse Fourier transform of the characteristic function

$$\int W(q, p) e^{i(kq\xi + kp\eta)}\, dq\, dp$$

and thus is nonnegative and represents a marginal distribution. Second, the Radon transform is a composition of the 2D-Fourier transform; and the 1D-inverse Fourier transform, thus it is invertible. The inverse Radon transform can be written as

$$W(q, p) = \int dQ\, d\xi\, d\eta\, RW(Q, \xi, \eta) e^{i(Q - q\xi - p\eta)}.$$

This means that knowing *projections* in all directions, one can reconstruct $W(x)$ from them by the inverse Radon transform. This property is widely used in computer tomography.

Due to the invertibility of Radon transform, the tomographic representation is equivalent to the Weyl symbol representation. In particular, the formula for the quantum mean takes the form (4):

$$\langle \hat{A} \rangle_\rho = \int dx\, A(x) W(x) = \int dQ\, d\xi\, d\eta\, \tilde{A}(\xi, \eta) RW(Q, \xi, \eta) e^{iQ},$$

where $\tilde{A}(\xi, \eta)$ is the Fourier inverse of $A(q, p)$ and $RW(Q, \xi, \eta)$ is the tomographic distribution corresponding to $W(x)$.

All of these representations finally lead to the same formula for the quantum Lyapunov exponent.

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