On the computation of quantum characteristic exponents

R. Vilela Mendes
Grupo de Física-Matemática, Complexo II - Univ. de Lisboa
Av. Gama Pinto, 2 - P1699 Lisboa Codex, Portugal

Ricardo Coutinho
Departamento de Matemática, Instituto Superior Técnico
Av. Rovisco Pais, 1096 Lisboa Codex, Portugal

Abstract
A quantum characteristic exponent may be defined, with the same operational meaning as the classical Lyapunov exponent when the latter is expressed as a functional of densities. Existence conditions and supporting measure properties are discussed as well as the problems encountered in the numerical computation of the quantum exponents. Although an example of true quantum chaos may be exhibited, the taming effect of quantum mechanics on chaos is quite apparent in the computation of the quantum exponents. However, even when the exponents vanish, the functionals used for their definition may still provide a characterization of distinct complexity classes for quantum behavior.

Keywords: quantum chaos, characteristic exponents

1 Introduction. Classical and quantum characteristic exponents.

A notion of quantum characteristic exponent has been introduced in Ref.[1], which has the same physical meaning as the corresponding classical quantity (the Lyapunov exponent). The correspondence is established by first
rewriting the classical Lyapunov exponent as a functional of densities and then constructing the corresponding quantity in quantum mechanics. The construction is explained in detail in Ref. [2], where the required functional spaces are identified and the infinite-dimensional measure theoretic framework is developed. Here we just recall the main definitions and emphasize some refinements concerning the support properties of the quantum characteristic exponents, which turn out to be relevant for the numerical computations of Sect. 2.

Expressed as a functional of admissible $L^1$—densities, the classical Lyapunov exponent is [2]

$$\lambda_v = \lim_{n \to \infty} \frac{1}{n} \log \left\| -v^i \frac{\partial}{\partial x^i} D_{\delta x} \left( \int d\mu(y) y P^n \rho(y) \right) \right\|$$

(1)

where $\rho$ is an initial condition density, $P$ the Perron-Frobenius operator, $x$ a generic phase-space coordinate, $v$ a vector in the tangent space, $\mu$ the invariant measure and $D_{\delta x}$ the Gateaux derivative along the generalized function $\delta_x$. The possibility to define Gateaux derivatives along generalized functions with point support and the need for a well-defined $\sigma$-additive measure in an infinite-dimensional functional space lead almost uniquely to the choice of the appropriate mathematical framework, that is, admissible densities are required to belong to a nuclear space. Being ergodic invariants, the Lyapunov exponents exist on the support of a measure. In the nuclear space framework, measures with support on generalized functions, which are in one-to-one correspondence with the usual measures in phase space, may be constructed by the Bochner-Minlos theorem [2].

To construct, in quantum mechanics, a quantity with the same operational meaning as (1) let $U^n$ (n continuous or discrete) be the unitary operator of quantum evolution acting on the Hilbert space $H$ and $\bar{X}$ a self-adjoint operator in $H$ belonging to a commuting set $S$. For definiteness $\bar{X}$ is assumed to have a continuous spectrum, to be for example a coordinate operator in configuration space. One considers, as in the classical case, the propagation of a perturbation $\partial_i \delta_x$, where by $x$ we mean now a point in the spectrum of $\bar{X}$.

$$v^i D_{\partial_i \delta_x} \left( U^n \Psi, \bar{X} U^n \Psi \right) = 2 \text{Re} \left. v^i \frac{\partial}{\partial x^i} \right|_{\delta_x} < \delta_x, U^{-n} \bar{X} U^n \Psi >$$

(2)
For the proper definition of the right-hand side of (2) one requires $\Psi \in E$ to be in a Gelfand triplet $E^* \supset H \supset E$

By $<\delta_x|$ or $<x|$ we denote a generalized eigenvector of $\tilde{X}$ in $E^*$. Notice also that $U^n$, being an element of the infinite-dimensional unitary group, has a natural action both in $E$ and $E^*$[4]. One obtains then the following definition of quantum characteristic exponent

$$\lambda_{v,x} = \limsup_{n \to \infty} \frac{1}{n} \log \left| \text{Re} \left( v^i \frac{\partial}{\partial x^i} <\delta_x, U^{-n}\tilde{X}U^n \Psi > \right) \right|$$

The support properties of this quantum version of the Lyapunov exponent have to be carefully analyzed. In Eq. (3), $\Psi$ defines the state which, in quantum mechanics, plays the role of a (non-commutative) measure[3]. The quantum exponent may depend on the state, but the measure that, as in the classical case, provides its support is not the state but a measure in the space of the perturbations of the initial conditions, that is, in the space where the Gateaux derivative operates. In the classical case these two measures coincide, in the sense that to which invariant measure in phase-space corresponds an infinite-dimensional measure in the space of generalized functions[2]. In the quantum case, however, the two entities are different, the second one being the measure on the spectrum of $\tilde{X}$ induced by the projection-valued spectral measure and the state, that is

$$\nu(\Delta x) = \langle \Psi, \int \Delta x dP_x \Psi \rangle$$

A particular case where an infinite-dimensional measure-theoretical setting, similar to the classical one, may be used to define the quantum exponents[2], is when the quantum evolution is implemented by substitution operators in configuration space, as in some sectors of the configurational quantum cat[4][6]. However this formulation is not very useful in general and the state plus spectrum-measure framework seems to be the one that has general validity. In this framework the following existence theorem holds

**Theorem:** Let $\tilde{X}$ be a self-adjoint operator, $E$ a test function space in a Gelfand triplet containing the generalized eigenvectors of $\tilde{X}$ in its dual $E^*$ and $\Psi \in E$. Then if $U^n \Phi \in E$ and $\tilde{X} \Phi \in E$ ($\forall \Phi \in E$, $\forall n \in \mathbb{Z}$) and the
following integrability condition is fulfilled

\[ \int d\nu(x) \log \left| \frac{\text{Re} v \partial x_i < x|U^{-1} \Phi >}{\text{Re} v \partial x_i < x|\Phi >} \right| < M \]  

(5)

\( \forall \Phi \in E \), the limit in Eq.(3) exists as a \( L^1(\nu) \)-function, that is, the average quantum characteristic exponent is defined for any measurable set in the support of \( \nu \).

Proof:

We write Eq.(3) as

\[ \lambda_v(x) = \limsup_{n \to \infty} \frac{1}{n} \sum_{k=0}^{n-1} \log \left| \frac{\text{Re} v \partial x_i < x|U^{-n+k} X U^{-n-k+1} \Phi >}{\text{Re} v \partial x_i < x|U^{-n+k-1} X U^{-n-k} \Phi >} \right| \]  

(6)

Then from the integrability condition (5) the integral of the sequence in the right-hand side of Eq.(6) is bounded and the Bolzano-Weierstrass theorem insures the existence of the \( \limsup \). Therefore \( \lambda_v(x) \) is well defined as a \( L^1(\nu) \)-function. \( \square \)

Notice that we really need the \( \limsup \) in the definition of the characteristic exponent because we have no natural \( U \)-invariant measure in \( E \) to be able, for example, to apply Birkhoff or Kingman’s theorem and prove \( \limsup = \liminf \). Also the sense in which the measure \( \nu \) provides the support for the quantum characteristic exponent is different from the classical ergodic theorems. We have not proven pointwise existence of the exponent a. e. in the support a measure. What we have obtained here is the possibility to define an average quantum characteristic exponent for arbitrarily small \( \nu \)-measurable sets.

Other definitions of characteristic exponents in infinite-dimensional spaces have been proposed by several authors\([8]\ [11] [11] [12] [13]\). They characterize several aspects of the dynamics of linear and non-linear systems. The definition discussed here, proposed for the first time in \([3]\), seems however to be the one that is as close as possible to the spirit of the classical definition of Lyapunov exponent.

Like the classical Lyapunov exponent the quantum analogue (3) cannot in general be obtained analytically. There is however a non-trivial example where it can. This is the configurational quantum cat introduced by
Weigert[6][7]. The phase space of this model is $T^2 \times \mathbb{R}^2$. A mapping similar to the classical cat operates as a quantum kick in the configuration space $T^2$, and the rest of the Floquet operator is a free evolution. This system has the appealing features of actually corresponding to the physical motion of a charged particle on a torus acted by an impulsive electromagnetic field and, as show by Weigert[7], to be exactly solvable.

The Floquet operator is

$$U = U_F U_K$$

$$U_F = \exp[-i \frac{T}{2} \tilde{p}^2]; \quad U_K = \exp[-\frac{i}{2}(\tilde{x} \cdot V \cdot \tilde{p} + \tilde{p} \cdot V \cdot \tilde{x})]$$

$U_F$ is a free evolution and $U_K$ a kick that operates in a simple manner on momentum eigenstates and on (generalized) position eigenstates

$$U_K |p\rangle = |M^{-1}p\rangle$$

$$U_K |x\rangle = |M x\rangle$$

$M$ being an hyperbolic matrix with integer entries and determinant equal to 1. The momentum has discrete spectrum, $p \in (2\pi\mathbb{Z})^2$.

To compute the quantum characteristic exponent (Eq.(3)), let the operator $\tilde{X}$ be

$$\tilde{X} = \sin(2\pi l \cdot x)$$

$l \in \mathbb{Z}^2$. This operator has the same set of generalized eigenvectors as the position operator $\tilde{x}$. To construct the measure $\nu$ (Eq.(4)) in the spectrum of the operator $\tilde{X}$ we cannot use the energy eigenstates $|P\alpha\rangle$ because they are not normalized. However all one requires is invariance of the measure, and using the (normalizable) momentum eigenstates one such measure is obtained.

$$\nu(A) = \langle p | \int_A dx | x\rangle \langle x | p\rangle$$

This invariant measure in this case happens to be simply the Lebesgue measure in $T^2$.

Defining

$$\gamma_n(x) = \langle x | U^{-n} \tilde{X} U^n | p\rangle$$

5
the result for the quantum characteristic exponent is

\[
\lambda_v = \limsup_{n \to \infty} \frac{1}{n} \log^+ \left| \text{Re} v^i \frac{\partial}{\partial x^i} \gamma_n(x) \right|
\]

\[
= \limsup_{n \to \infty} \frac{1}{n} \log^+ \left| v^i (2\pi M^n l)_i \{ \cos \theta_n(p,l,x) + \cos \theta_n(p,-l,x) \} \right|
\]

with

\[
\theta_n(p,l,x) = \frac{T}{2} \left( \sum_{k=0}^{n-1} (M^{-k}p)^2 + \sum_{k=0}^{n-1} (M^k(2\pi l + M^{-n}p))^2 + x \cdot (2\pi M^n l + p) \right)
\]

For the lim sup the cosine term plays no role and finally

\[
\lambda_v = \lim sup \frac{1}{n} \log \left| v^i (M^n l)_i \right|
\]

The characteristic exponent is then determined from the eigenvalues of the hyperbolic matrix \( M \) and is the same everywhere in the support of the measure \( \nu \). If \( \mu_1, \mu_2 \) (\( \mu_1 > \mu_2 \)) are the eigenvalues of \( M \), one obtains \( \lambda_v = \log \mu_1 \) for a generic vector \( v \) and \( \lambda_v = \log \mu_2 \) iff \( \nu \) is orthogonal to the eigenvector associated to \( \mu_1 \). Hence, in this case, one obtains a positive quantum characteristic exponent whenever the corresponding classical Lyapunov exponent is also positive.

This exact example will be used in Sect.2 as a testing ground for the numerical algorithm and an illustration of the kind of precision problems and support properties to be expected when computing quantum characteristic exponents.

In the numerical calculation of the quantum characteristic exponents two delicate points are identified. The first is that the calculation requires a high degree of precision, because, if the exponent is positive, the derivative of \( U^{-n} \tilde{X} U^n \Psi(x) \) grows very rapidly with \( n \). Therefore in the positive exponent case acceptable statistics is only obtained by taking average values over the configuration space. Second, if the situation is as in the classical case where different invariant measures coexist in phase space, the quantum exponent may depend on the state \( \Psi \) used to define the measure \( \nu \) in the spectrum of \( \tilde{X} \). Therefore, in all rigor, one should first construct stationary states and then study the \( \Psi \)-dependence of the quantum exponent. Such study has not yet been carried out and, in the calculations below, a flat wave function is used as the initial state.
2 Numerical computation of quantum characteristic exponents

For kicked quantum systems corresponding to the Hamiltonian
\[ H = H_0 + V(x) \sum_j \delta(t - j\tau) \] (16)
the Floquet operator is
\[ U = e^{-iV(x)} e^{-i\tau H_0(\frac{\omega}{\Delta t})} \] (17)
in units where \( \hbar = 1 \). For the computation of the action of \( U \) on a wave function \( \psi(x) \), a fast Fourier transform algorithm \( F \) and its inverse \( F^{-1} \) are used
\[ U\psi(x) = e^{-iV(x)} F^{-1} e^{-i\tau H_0(ik)} F\psi(x) \] (18)
In this way one obtains a uniform algorithm for any potential. In the configurational quantum cat, Eq.(8), the computation is similar with the multiplicative kick \( e^{-iV(x)} \) replaced by the substitution operator
\[ \psi(x) \rightarrow \psi(M^{-1}x) \] (19)
The quantum characteristic exponent is obtained from the calculation of
\[ \partial_x U^{-n} \tilde{X} U^n \psi(x) \] (20)
in the limit of large \( n \). The precision of the algorithm is checked by insuring that
\[ \left| (U^{-n} U^n - 1) \psi(x) \right| < \epsilon \] (21)
for a small \( \epsilon \), and that the finite difference used to compute the derivative in (20) does not approach the maximum possible value allowed by the discretization.

2.1 The configurational quantum cat

Here the configuration space is the 2-torus \( T^2 \), the Floquet operator is the one of Eq.(8), and the kick is a substitution operator with matrix
\[ M = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \] (22)
Numerically we have computed the quantities
\[
\frac{1}{n} \langle D_n - D_0 \rangle = \frac{1}{n} \left\langle \log \frac{\left| Re v^i \frac{\partial}{\partial x} \left( U^{-n} \tilde{X} U^n \Psi \right)(x) \right|}{\left| Re v^i \frac{\partial}{\partial x} \left( \tilde{X} \Psi \right)(x) \right|} \right\rangle_{T^2}
\]  
(23)
\tilde{X} being the operator in (11). The initial wave function is \( \Psi(x) = 1 \) and the average is taken over the whole of configuration space. It turns out that, in this case, the derivative in the numerator of (23) grows so fast at some points that one reaches, after a few iterations, the maximum difference (2 in this case) for the wave function at two nearby points in the discretization grid. When this happens the calculation cannot be reliably taken to higher \( n \) with that discretization. In the numerical calculation of the classical Lyapunov the computation becomes a local evaluation at each step by rescaling the transported tangent vector. Here, because of the linearity of matrix elements and quantum evolution, a similar procedure is not possible and one has to carefully control the growth of the quantities in (23). To improve statistics the average over configuration space has been taken. This can be safely done in this case because we know exactly the supporting measure (12), but in general there will be no guarantee that the supporting spectral measure is uniform. In any case average quantities like (23) are exactly what one expects to be able to compute reliably.

Fig. 1 shows the evolution of \( \frac{1}{n} \langle D_n - D_0 \rangle \) obtained with a discretization grid of 292681 points in the unit square, for two different directions \( \nu \). The calculation was interrupted when the local finite differences reached one half of the maximum. The lines are fits to the points constrained to approach the same value at large \( n \). The resulting numerical estimate for the largest quantum characteristic exponent is 0.95. The exact value obtained from (15) is 0.9624.

### 2.2 Quantum kicked rotators

The configuration space is the circle \( S^1 \),
\[
V(x) = q \cos(2\pi x)
\]  
(24)
\( x \in [0, 1) \) and for \( H_0 \) the following two possibilities were explored
\[
H_0^{(1)} = -\frac{1}{2\pi} \frac{d^2}{dx^2}
\]
\[
H_0^{(2)} = -2\pi \cos \left( \frac{1}{2\pi i} \frac{d}{dx} \right)
\]  
(25)
The operator $\tilde{X}$ is

$$\tilde{X} = \sin(2\pi x)$$

(26)

The quantity that is numerically computed is

$$\langle D_n \rangle = \left\langle \log \left| \text{Re} \left( \frac{\partial}{\partial x} \left( U^{-n} \tilde{X} U^n \Psi \right) (x) \right) \right| \right\rangle$$

(27)

and, in all cases, one starts from a flat initial wave function. In both cases and for the very many values of $q$ that were studied, this quantity seems either to stabilize or to have a very small rate of growth for large $n$. Fig.2, for example, shows the results for the $H_0^{(1)}$ case with $\tau = \frac{\sqrt{5}}{2}$ and $q = 5$. The (numerical) conclusion is that the quantum characteristic exponent vanishes. This conclusion does not seem to be a numerical artifact because the discretization grid for the fast Fourier transform has always been chosen sufficiently small to insure a small local finite difference for all iterations. For example in the example shown in Fig.2, the grid has 4096 points which keeps observed local differences below 0.1. Also the vanishing of the quantum characteristic exponent in quantum kicked rotators is not dependent on the phenomena of localization because also for quantum resonances it may exactly be shown to vanish [4].

In Fig.2 $\langle D_n \rangle$ seems to tend to a constant at large $n$. In other cases very slow rates of growth are observed. This is shown in Figs.3a,b for the $H_0^{(2)}$ case with $\tau = \frac{\sqrt{5}}{2}$ and $q = 11$.

3 Conclusions

Both the classical Lyapunov exponent [4] and its quantum counterpart [3], measure the exponential rate of separation of matrix elements of $\tilde{X}$ when the density (or the wave function) suffers a $\delta'_x$ perturbation, $x$ being a point in the spectrum of $\tilde{X}$. The configurational quantum cat example shows that there are instances of true quantum chaos, in the sense of exponential growth of the matrix element separation. However, as the numerical study of the quantum kicked rotators seems to show, exponential growth may be rather exceptional in quantum mechanics. Furthermore the taming effect of quantum mechanics on exponential chaos goes deeper than the phenomenon of localization, because also for quantum resonances, where no localization is present, the quantum characteristic exponent vanishes.
Although distinct from one another, all known ways that now exist to approach the problem of quantum chaos, seem to agree in one point, namely that quantum mechanics has a definite taming effect on chaos. This is now probably the main issue in quantum chaos, not only from the theoretical point of view, but also in the context of quantum control. Even if quantum characteristic exponent, as defined in (3) might be zero in most quantum systems, the rate of growth index \( D_n \) or its average \( \langle D_n \rangle \) might still be useful as a characterization of quantum dynamics because, even if weaker than exponential, a growth of this quantity would still be an indication of sensitivity to initial conditions. In particular, as suggested by the numerical results, subexponential rates of growth might characterize distinct complexity classes of quantum evolution.

### 4 Figure captions

Fig.1 - Calculation of \( \frac{1}{n} \langle D_n - D_0 \rangle \), Eq.(23), in the configurational quantum cat for two orthogonal directions \( \nu \) and a fit constrained to the same limit at large \( n \).

Fig.2 - \( \langle D_n \rangle \), Eq.(27), for the quantum standard map at \( q = 5, \tau = \frac{5}{2} \).

Fig.3 - (a) \( \langle D_n \rangle \), Eq.(27), for a kicked rotator with kinetic Hamiltonian \( H_0^{(2)} \) at \( q = 11, \tau = \frac{5}{2} \); (b) the same scaled by \( \log(\log(n+1)) \).

### References

[1] R. Vilela Mendes; Phys. Lett. A171, 253 (1992).

[2] R. Vilela Mendes; in *Chaos - The Interplay between Stochastic and Deterministic Behaviour*, page 273, P. Garbaczewski and A. Weron (Eds.), Springer Lecture Notes in Physics no. 457, Springer, Berlin 1995.

[3] I. M. Gelfand and N. Ya. Vilenkin; *Generalized functions*, vol. 4, Academic Press, New York 1964.

[4] T. Hida; *Brownian Motion*, Springer, Berlin 1980.

[5] A. Connes; *Noncommutative geometry*, Academic Press 1994.
[6] S. Weigert; Z. Phys. B - Condensed Matter 80, 3 (1990).

[7] S. Weigert; Phys. Rev. A48, 1780 (1993).

[8] D. Ruelle; Ann. Math. 115, 243 (1982).

[9] R. Vilela Mendes; J. Phys. A: Math. Gen. 24, 4349 (1991).

[10] F. Haake, H. Wiedemann and K. Zyczkowski; Ann. Physik 1, 531 (1992).

[11] K. Zyczkowski, H. Wiedeman and W. Slomczynski; Vistas in Astronomy 37, 153 (1993).

[12] W. Majewski and M. Kuna, J. Math. Phys. 34, 5007 (1993).

[13] G. G. Emch, H. Narnhofer, W. Thirring and G. L. Sewell; J. Math. Phys. 35, 5582 (1994).
Fig. 2

mean(Dn)

n
Fig. 3a

![Graph showing the mean(Dₙ) vs. n]
mean(Dn)/\log(\log(n+1))

Fig. 3b