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Sensitive dependence in quantum systems : Some examples and results

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Abstract

Considering the time evolution of perturbations of the wave function along directions of the δ' type one obtains a notion of quantum sensitive dependence and quantum characteristic exponent resembling the corresponding classical quantities. These notions are proposed as a tool to characterize quantum chaos.

From the study of some examples one concludes that quantum sensitive dependence and delocalization of the wave functions are independent questions.

The numerical reversibility of classically chaotic quantum systems is discussed in the quantum sensitive dependence context.

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1. Quantum sensitive dependence and characteristic exponents

Chaos in classical mechanics is closely related to the notion of sensitive dependence on initial conditions, that is to the existence of at least one positive Lyapunov exponent. To attempt a similar characterization of quantum chaos, the notion of ***quantum sensitive dependence*** has been introduced[1,2]. This we recall briefly here.

For some initial wave function $\psi(0)$, at $t=0$, one considers an infinitesimal deformation

$$\psi(0) \to \psi_\delta(0) \;=\; \psi(0) \;+\; \delta\,\phi(0) \tag{1.1}$$

The separation in time of nearby initial conditions is then measured by the expectation value of a self-adjoint operator $\mathcal{A}$

$$\Delta_\delta(t) \;=\; (\psi_\delta(t),\mathcal{A}\psi_\delta(t)) \;-\; (\psi(t),\mathcal{A}\psi(t)) \;\simeq\; 2\,\delta\,\mathrm{Re}(\phi(t),\mathcal{A}\psi(t)) \tag{1.2}$$

We then say that there is $\mathcal{A}-$***sensitive dependence at the state*** ψ if there is at least one ϕ for which $\lim\limits_{\delta\to 0}\left\|\dfrac{\Delta_\delta(t)}{\Delta_\delta(0)}\right\|$ is unbounded in time. Also, whenever the following limit exists

$$\lambda_{\mathcal{A},\phi} \;=\; \lim_{T\to\infty}\frac{1}{T}\ln\left\|\mathrm{Re}(\phi(T),\mathcal{A}\psi(T))\right\| \tag{1.3}$$

it is called a $\mathcal{A}-$***quantum characteristic exponent*** at ψ. Notice that with these definitions a quantum system may be $\mathcal{A}-$sensitive dependent and the quantum characteristic exponent be zero, if the rate of growth of $\left\|\dfrac{\Delta_\delta(t)}{\Delta_\delta(0)}\right\|$ is slower than exponential.

If $\mathcal{A}$ is defined everywhere in Hilbert space, by the Hellinger-Toeplitz theorem it is a bounded operator. Hence if the vector ϕ, that defines the deformation direction, belongs to the Hilbert space there cannot be any $\mathcal{A}-$sensitive dependence along ϕ and $\lambda_{\mathcal{A},\phi}=0$. Therefore for deformation directions ϕ in Hilbert space $\mathcal{A}-$sensitive dependence is only possible if $\mathcal{A}$ is an unbounded operator. In contrast, for the classical notion of Lyapunov exponent, bounded systems may have positive Lyapunov exponents even if the separation of the orbits is measured by a bounded variable. This suggests that to obtain in quantum mechanics a notion resembling the classical Lyapunov exponent, ϕ should not be limited to Hilbert space vectors. We therefore generalize here the notion of $\mathcal{A}-$quantum characteristic exponent to

$$\lambda_{\mathcal{A},\{\phi_n\}} = \lim_{T\to\infty} \frac{1}{T} \lim_{n\to\infty} \ln\left\| \mathrm{Re}(\phi_n(T),\mathcal{A}\psi(T)) \right\| \tag{1.4}$$

where ϕ_n is a sequence of functions that may converge to an element outside Hilbert space (in $\mathcal{S}'$ for example).

To find what kind of deformation directions, in the space of functions, correspond to the classical notion of Lyapunov exponent, consider the definition of this exponent in terms of classical densities. We consider the case of one variable and then generalize to arbitrary number of variables. Let $\rho(x)$ be the reference density for a system defined in the interval [a,b] and $\bar{\rho}_n(x)$ a family of deformed densities

$$\bar{\rho}_n(x) - \rho_n(x) = \epsilon\, \eta_n(x) \tag{1.5}$$

($\int \bar{\rho}_n = \int \rho = 1$) . We now want to follow the separation in time of the two densities by computing the average value of the position

$$(\Delta_n x)_k = \int x\, \{f^k \bar{\rho}_n(x) - f^k \rho(x)\}\, dx \tag{1.6}$$

From the Frobenius-Perron operator[3] $f\rho(x) = \sum_i \rho(f^{-1}x)_i \frac{1}{\left\| f'(f^{-1}x)_i \right\|}$ one obtains, by change of variables

$$(\Delta_n x)_k = \int f^k(x)\, \{\bar{\rho}_n(x) - \rho(x)\}\, dx = \epsilon \int f^k(x)\, \eta_n(x)\, dx \tag{1.7}$$

To obtain the Lyapunov exponent $\lim_{k\to\infty} \frac{1}{k} \ln\left\| f^{k\prime}(x_o) \right\|$ from

$$\lim_{k\to\infty} \frac{1}{k} \lim_{n} \ln \left\| \frac{(\Delta_n x)_k}{(\Delta_n x)_0} \right\| \tag{1.8}$$

one must now choose

$$\lim_{n} \eta_n(x) = \delta'(x - x_o) \tag{1.9}$$

Therefore to extract the Lyapunov exponent from the behavior of the densities the deformation direction no longer lies in Hilbert space. For higher dimensions the deformation directions to consider (again in $\mathcal{S}'$) are directional derivatives of the δ. Notice that in (1.8) it is essential to consider first the limit in n and then the limit in k. This parallels the fact that in the classical definition of the Lyapunov exponent

$$\lim_{k\to\infty} \frac{1}{k} \lim_{\Delta x\to 0} \ln \left\| \frac{d(\Delta x,k)}{d(\Delta x,0)} \right\| \tag{1.10}$$

the limit $\Delta x \to 0$ must also precede the $k \to \infty$ limit.

For quantum mechanics a similar modification of the initial probability density will be obtained if one considers the following deformations of the initial wave function

$$\psi \to \psi + \epsilon\, \partial_1 \delta(x - x_0)$$

being understood that whenever necessary the calculations are performed with a sequence ϕ_n of functions approaching the directional derivative of the delta. Also the $\epsilon \to 0$ limit should be taken in such a way that terms of order ϵ^2 are negligible for all n.

We now analyze some examples.

2. The 4-dimensional Arnold's cat

The classical Arnold's cat[4] is the following automorphism of the 2-torus

$$(x_1', x_2') = f(x_1, x_2) = (x_1 + x_2, x_1 + 2x_2) \qquad (\text{mod. } 1) \tag{2.1}$$

inducing in the covering plane $\mathbf{R}^2$ the linear mapping

$$\tilde{f} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} \tag{2.2}$$

The motion in the covering plane $\mathbf{R}^2$ or even in $S^1 \times \mathbf{R}$ is a simple transient motion with orbits flying away to infinity. It is the folding of both coordinates into a torus that is responsible for the mixing properties.

If one of the coordinates is interpreted as the configuration coordinate and the other as the momentum, the classical Arnold's cat is the time-one map of the following kicked Hamiltonian

$$H = \frac{x_2^2}{2} - \frac{x_1^2}{2} \sum_{n \in \mathbf{Z}} \delta(t - n) \tag{2.3}$$

The physical interpretation of this Hamiltonian is however crucial when one quantizes the theory. If it is interpreted as describing the motion of a periodically kicked particle living on a circle, then x_2 (the conjugate momentum) is unbounded and the quantum theory has a transient absolutely continuous spectrum and no mixing properties. If one imposes periodicity on x_2 as well as on x_1, this has the effect of introducing a cut-off on momentum. When going to the quantum theory, in the same way as the periodic boundary conditions on x_1 imply that only a discrete set of momenta are allowed, so the

x_2-periodicity implies discreteness in x_1. The effective quantum space is therefore reduced to a grid of N^2- $\left(\frac{1}{h}\right)^2$ points. In general, quantization of a system living in a continuous space does not, by itself, discretize the space. Periodicity in the conjugate momentum is therefore seen to be a condition which, when imposed in addition to quantization, naturally produces a quantum system qualitatively different from the classical one. It is this cut-off in momentum that underlies the claimed failure of the correspondence principle in the work of Ford, Mantica and Ristow[5].

There are however other physical interpretations of the Arnold's cat map. The classical map may be considered as the stroboscopic map of the $p_{x_1} = p_{x_2} = 0$ sector of one of the following Hamiltonians

$$H_1 = \frac{p_{x_1}^2}{2} + \frac{p_{x_2}^2}{2} + x_2\, p_{x_1} + x_1\, p_{x_2} \sum_{n \in \mathbf{Z}} \delta(t - nT) \tag{2.4a}$$

$$H_2 = \frac{p_{x_1}^2}{2} + \frac{p_{x_2}^2}{2} + \{x_2\, p_{x_1} + (x_1 + x_2)\, p_{x_2}\} \sum_{n \in \mathbf{Z}} \delta(t - nT) \tag{2.4b}$$

which describe (the small charge limit) of a charged particle constrained to move in the x_1x_2-torus under the influence of a time-dependent electromagnetic field. For the quantum theory of the Hamiltonian H_2, Weigert[6] has shown that for particular values of the kicking period T, the free evolution is the identity operator and the Floquet operator acting on the wave functions coincides with the classical evolution.

Here, without making reference to any particular Hamiltonian, we simply specify a *4-dimensional Arnold's quantum cat* as the quantum theory defined by the Floquet operator U

$$\psi(x_1,x_2) \to \psi'(x_1,x_2) = \psi\left(f^{-1}(x_1,x_2)\right) = U\, \psi(x_1,x_2) \tag{2.5}$$

Eq.(2.5) defines a unitary evolution. Operating with $p_{x_i} = \frac{\hbar}{i}\frac{\partial}{\partial x_i}$, the time evolution of the momenta is obtained and (2.5) completely defines a quantum theory. Notice however that, except in special resonance conditions, the dynamics is different from the one associated with the Hamiltonians (2.4).

The nth iterate of the map (2.2) and its inverse, in the covering space, are

$$\tilde{f}^{\,n} = \frac{1}{\sqrt{5}} \begin{bmatrix} \omega^{-2n+1} + \omega^{2n-1} & -\omega^{-2n} + \omega^{2n} \\ -\omega^{-2n} + \omega^{2n} & \omega^{-2n-1} + \omega^{2n+1} \end{bmatrix} \tag{2.6a}$$

$$\tilde{f}^{-n} = \frac{1}{\sqrt{5}} \begin{bmatrix} \omega^{2n+1} + \omega^{-2n-1} & -\omega^{2n} + \omega^{-2n} \\ -\omega^{2n} + \omega^{-2n} & \omega^{2n-1} + \omega^{-2n+1} \end{bmatrix} \tag{2.6b}$$

where $\omega = \frac{1+\sqrt{5}}{2}$.

Consider doubly periodic wave functions $\psi(x)$ and a sequence of functions $\phi_n(x)$ approaching a directional derivative of the delta

$$\phi_n(x) \to \epsilon\, \partial_j\, \delta(x - x_o)$$

which may be represented in the basis $\left\{e^{ip.x};\ p_1, p_2 \in Z\right\}$. Computing $(U^k \phi_n\ ,\ x_i\ U^k \psi)$

$$\int \phi_n\left(f^{-k}(x)\right)\ x_i\ \psi\left(f^{-k}(x)\right)\ d^2x = \int \phi_n(x)\ \left\{(\tilde{f}^k x)_i - m_i(x,k)\right\}\ \psi(x)\ d^2x$$

The arguments of ϕ_n and ψ are computed using the matrices (2.6) mod.1. This is explicitly represented in the second integral where $m_i(x,k)$ is the integer to be subtracted from $(\tilde{f}^k x)_i$ to obtain a value between zero and one. When x_o is a generic point that does not coincide with the discontinuities introduced by $m_i(x,k)$ and the sequence ϕ_n tends to $\epsilon\partial_j\ \delta(x - x_o)$, the above integral is simply evaluated by differentiation of $(\tilde{f}^k x)_i$. Then

$$\lim_{k\to\infty} \frac{1}{k} \lim_{\substack{n\to\infty \\ \epsilon\to 0}} \ln \left\| \frac{\mathrm{Re}(U^k \phi_n,\ x_i\ U^k \psi)}{\mathrm{Re}(\phi_n,\ x_i\ \psi)} \right\| = \ln \omega^2 \tag{2.7}$$

which coincides with the value of the classical Lyapunov exponent.

3. Kicked motions on the circle and on the line

The first Hamiltonian to be considered in this Section is

$$H_1 = \alpha\, p + V_1(x) \sum_Z \delta(t - n) \qquad x \in [0,1) \tag{3.1}$$

to which corresponds the classical map

$$x_{n+1} = x_n + \alpha \qquad p_{n+1} = p_n - V'(x_n) \tag{3.2}$$

Models of this type have been used by several authors[7-10] in the context of the theory of incommensurate crystals. The conditions on α and $V(x)$ that correspond to point-like or to absolutely continuous spectrum of the Floquet operator have been extensively characterized[11]. The Floquet operator associated to (3.1) is

$$U = e^{-\alpha \frac{d}{dx}}\ e^{-iV_1(x)} \tag{3.3}$$

which acts on the wave functions by

$$U^k \psi(x) = e^{-i\sum_{j=0}^{k-1} V_1(x-j\alpha)} \psi(x-k\alpha) \tag{3.4}$$

Both $\psi(x)$ and $V(x)$, in the above equation, are assumed to be periodically extended outside the interval $[0,1)$. The computation of the matrix element $\left(U^k\delta'(x-x_0), xU^k\psi(x)\right)$ is straightforward and one obtains

$$\lim_{k\to\infty} \frac{1}{k} \ln \left\| \frac{\mathrm{Re}(U^k\delta', x\, U^k\psi)}{\mathrm{Re}(\delta', x\, \psi)} \right\| = 0 \tag{3.5}$$

Choosing other operators $\mathcal{A}$ to define the separation (1.2) of the wave functions, the result is similar. For example if $\mathcal{A} = -\frac{\partial^2}{\partial x^2}$ (the free kinetic energy) the matrix elements grow at most quadratically in time and the quantum characteristic exponent vanishes.

This example also shows that the problem of localization or delocalization of the wave functions and quantum sensitive dependence are different questions. Localization of the wave functions of time-periodic Hamiltonians is related to the nature of the spectrum of the Floquet operator, localization corresponding to the point spectrum and delocalization (local decay) to the continuous spectrum[12,13]. It is known[11] that, for the Hamiltonian (3.1), the spectrum of the Floquet operator may be either point-like or absolutely continuous depending on α and $V(x)$. However in both cases the quantum characteristic exponent vanishes. The same situation is found for other kicked Hamiltonians. For example for the kicked rotator

$$H_1 = -\frac{\alpha}{2\pi}\frac{\partial^2}{\partial x^2} + V_2(x) \sum_{\mathbb{Z}} \delta(t-n) \qquad x \in [0,1) \tag{3.7}$$

with $V_2(x) = k\cos(2\pi x)$, it is known[14] that for the situation of quantum resonance ($\alpha = \frac{p}{q}$) the rotator energy grows quadratically in time for large times and the spectrum of the Floquet operator is continuous. However this does not necessarily imply non-vanishing quantum characteristic exponents. For example for the fundamental quantum resonance (α=integer) the evolution is simply

$$U^n\psi(x) \to e^{-i\,n\,k\cos(2\pi x)}\,\psi(x)$$

and both the $x-$ and $\frac{\partial^2}{\partial x^2}-$quantum characteristic exponents are zero.

Let now the Hamiltonian (3.7) be defined on the whole line and $V_2(x) = \frac{\gamma}{2}x^2$, ($\gamma > 0$), describing a free motion on the line with periodic harmonic kicks. In this case the Floquet operator is

$$U = e^{i\frac{\gamma}{2}x^2}\, e^{i\frac{\alpha}{2\pi}\frac{d^2}{dx^2}}$$

and the matrix element $\left(U^k\phi_n, x\, U^k\psi\right) \to \epsilon\left(\delta', U^{-k}xU^k\,\psi\right)$ may be computed explicitly.

One obtains

$$U^{-k}\, x\, U^{k} = A_k\, x + B_k\left(-i\,\frac{d}{dx}\right) \tag{3.8}$$

with

$$A_k = \frac{z}{2}\sum_{p\ \mathrm{odd}}\binom{k}{p}\left(1-\frac{z}{2}\right)^{k-p}\left(\frac{z^2}{4}-z\right)^{\frac{p-1}{2}} + \sum_{p\ \mathrm{even}}\binom{k}{p}\left(1-\frac{z}{2}\right)^{k-p}\left(\frac{z^2}{4}-z\right)^{\frac{p}{2}}$$

$$B_k = -\frac{z}{\gamma}\sum_{p\ \mathrm{odd}}\binom{k}{p}\left(1-\frac{z}{2}\right)^{k-p}\left(\frac{z^2}{4}-z\right)^{\frac{p-1}{2}}$$

where $z = \gamma\,\frac{\alpha}{\pi}$

The matrix element $\left(\delta',\, U^{-k} x U^{k}\, \psi\right)$ is now obtained by differentiation of (3.8). One has two cases which correspond to the classical elliptic and hyperbolic situations. In the elliptic case ($z < 4$)

$$\lim_{k\to\infty}\frac{1}{k}\ \ln\left\|\frac{\mathrm{Re}(U^{k}\delta',\, x\, U^{k}\psi)}{\mathrm{Re}(\delta',\, x\,\psi)}\right\| = 0$$

and the hyperbolic case ($z > 4$)

$$\lim_{k\to\infty}\frac{1}{k}\ \ln\left\|\frac{\mathrm{Re}(U^{k}\delta',\, x\, U^{k}\psi)}{\mathrm{Re}(\delta',\, x\,\psi)}\right\| = \ln\left\|1-\frac{z}{2}-\sqrt{\frac{z^2}{4}-z}\right\|$$

which coincides with the classical results. The elliptic and the hyperbolic cases correspond[15] respectively to point-like and to continuous spectrum. This is therefore a case where the continuous spectrum appears together with positive quantum exponents although, as emphasized above, the two questions seem to be independent. On the other hand, in the examples that were studied, the quantum characteristic exponents are closely related to the corresponding classical quantities. Why is it then that the quantum dynamics of classically chaotic systems looks so different from the classical behavior. One possible reason is discussed in the next section.

4. Numerical reversibility of quantum evolution

The exponential separation of the orbits in classical chaotic systems implies that reversal of the time evolution cannot, in practice, be carried out in computer experiments. The numerically computed time evolution reproduces backwards the history of the system only for a short time, that is, the memory of the initial state is quickly lost because of the exponential amplification of the round off computer errors.

For this reason the lack of numerical reversibility became to be thought of as the true mark of dynamical chaos.

Numerical experiments[16,17] on time reversal of the quantum evolution of classically chaotic systems have however shown that the evolution can be traced back to the initial state just by reversing the phases in the Fourier expansion of the wave function. Furthermore, that reversibility is largely unaffected by a small change in the phases before reversal. The discussion of quantum sensitive dependence in the preceding sections may shed some light into this question. In fact there is a remarkable difference between the effect of round off errors in the usual computer simulations of classical and of quantum systems.

In simulations of classical systems one follows the phase-space orbits and the computer simulations essentially explore all directions in phase-space, both the stable and the unstable ones (those with positive Lyapunov exponents). For quantum systems the simulations compute a finite number of Fourier coefficients of the wave function in some basis. Now, as we have seen above, exponential growth of the matrix elements of bounded operators can only be obtained for deformations of the wave function along directions outside Hilbert space, namely of the δ' type. For a $\delta'(x-x_0)$ in the circle the n-th Fourier coefficient is $i\,n\,e^{-inx_0}$. The coefficient grows with the order of the Fourier mode and no finite truncation can correctly approximate $\delta'(x-x_0)$. An error in a computer simulation is an error in a finite number of Fourier modes, hence it is a deformation of the wave function along a direction inside Hilbert space. Therefore it is a deformation along a stable direction for which the characteristic exponent vanishes. Even if one considers unbounded operators (like the kinetic energy) to measure orbit separation in (1.2), it is found that the deformations along Hilbert space vectors ϕ lead in general at most to polynomial growth of the matrix elements in (1.3). Therefore there might be $\mathcal{A}$-sensitive dependence, according to the definition in Section 1, but the ϕ-characteristic exponent vanishes.

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