QUANTUM CHAOS: A DECOHERENT DEFINITION.

WOJCIECH HUBERT ZUREK$^{(1)}$ AND JUAN PABLO PAZ$^{(1,2)}$

(1): Theoretical Astrophysics, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

(2): Departamento de Física, Facultad de Ciencias Exactas y Naturales, Pabellón 1, Ciudad Universitaria, 1428 Buenos Aires, Argentina

ABSTRACT: We show that the rate of increase of von Neumann entropy computed from the reduced density matrix of an open quantum system is an excellent indicator of the dynamical behavior of its classical hamiltonian counterpart. In decohering quantum analogs of systems which exhibit classical hamiltonian chaos entropy production rate quickly tends to a constant which is given by the sum of the positive Lyapunov exponents, and falls off only as the system approaches equilibrium. By contrast, integrable systems tend to have entropy production rate which decreases as $t^{-1}$ well before equilibrium is attained. Thus, behavior of quantum systems in contact with the environment can be used as a test to determine the nature of their hamiltonian evolution.
1. INTRODUCTION

Ever since the inception of quantum theory, the issue of the correspondence between quantum and classical has been at the center of interest. Perhaps the best known (and most durable!) problem arises in the context of measurements. The difficulty of representing the Universe as a whole – including us, the observers – by means of quantum theory has been known to the forefathers of quantum physics, and (in spite of the significant recent progress) continues to be hotly debated. The problem of the correspondence between the quantum and the classical in quantum analogs of systems which classically exhibit dynamical chaos has come into focus within the past two decades. It is perhaps best illustrated by the fact that, in course of the hamiltonian evolution, quantum and classical versions of the same system begin to exhibit significant discrepancies between the expectation values of the same quantity on a relatively short timescale:

\[ t_\chi \propto \lambda^{-1} \log(\chi \delta p/\hbar). \]  

Above \( \lambda \) is the Lyapunov exponent, \( \chi \) is the scale over which the potential becomes significantly nonlinear, and \( \delta p \) characterizes the initial spread of the wavepacket in the units of momentum.

This timescale is only logarithmically dependent on the value of the Planck constant \( \hbar \). Thus, it is uncomfortably short, even for macroscopic systems: If one were to take this prediction on the face value one would anticipate that in our Universe quantum chaotic systems should stop obeying classical laws after a few dynamical timescales (which is typically the order of the inverse Lyapunov exponent \( \lambda^{-1} \)). By contrast, quantized regular (integrable) systems tend to follow predictions of classical mechanics for much longer time – on a timescale of the order of \((1/\hbar)^\beta\) where \( \beta \) is some (positive) characteristic power. This failure of the correspondence principle for chaotic systems has even led some to wonder whether quantum theory can be the fundamental theory of our Universe which – after all – seems to follow classical mechanics at the macroscopic level.

The purpose of this paper is to provide a brief summary of the relevant aspects of the process of decoherence – which was introduced to deal with the transition from quantum to classical in quantum measurements – and to show how it helps resolve the problem of quantum–classical correspondence in the context of chaos. As an important corollary of this discussion we will conjecture a simple method to diagnose chaos in the fully quantum system. We shall base it on the behavior of the von Neumann entropy.
production rate of systems coupled to an environment. In cases where the classical system is chaotic, von Neumann entropy is conjectured to increase at a rate given by Lyapunov exponents in its decoherring quantum analog. By contrast, in quantum analogs of regular systems entropy will grow at a rate which will asymptotically tend to zero well before the system reaches equilibrium.

What is remarkable about this result\textsuperscript{11} is that the entropy production rate – following the initial onset of decoherence which occurs on a *decoherence timescale*\textsuperscript{12} which is essentially independent of the system’s self-hamiltonian, but dependent on the strength and nature of the coupling with the environment\textsuperscript{13} and on the form of the initial state\textsuperscript{9,14} – tends to be dictated by the dynamics of the system rather than by the type or the strength of the coupling. Independence from the strength and nature of the coupling holds for a wide range of parameters in spite of the fact that the ultimate cause of irreversibility is precisely the coupling with the environment. This behavior mirrors classical intuition about the nature of chaotic systems: Their evolution is – in contrast to regular systems – unpredictable. We show that this unpredictability carries over into the quantum domain, provided that systems which are *open* are investigated. This result can be therefore regarded as an additional indication that the correspondence between quantum and classical dynamics should be sought only with the assistance of environment – induced superselection, the consequence of the process of decoherence. Furthermore, entropy production rate in a decoherring quantum system can be regarded as a diagnostic tool: Rate of increase of entropy can distinguish chaotic and regular quantum evolutions, thus providing a completely quantum definition of quantum chaos.

2. DECOHERENCE

Decoherence and its relation with quantum measurement are not the main subjects of this paper. We shall summarize decoherence only very briefly with the eye on its significance to the subject of the transition from quantum to classical in the context of quantum chaos. A more complete review can be found elsewhere\textsuperscript{15,16}

Decoherence is the process of loss of (phase) coherence by the system caused by the interaction with the external or internal degrees of freedom which cannot be followed by the observer and are summarily called ‘the environment’. Different states in the Hilbert space of the system of interest show various degrees of susceptibility to decoherence. States
which are least susceptible (i.e., take longest to decohere) form the preferred basis (also known as the pointer basis, in the context of quantum measurement)\textsuperscript{9,15,16,17}.

Preferred states are singled out by the interaction between the system and the environment. In idealized discussions of quantum apparatus, complete immunity to decoherence can be guaranteed for the eigenstates of the pointer observable which commutes with the total hamiltonian (i.e., self hamiltonian plus the interaction hamiltonian). Hence, pointer observable is conserved in spite of the interaction with the external degrees of freedom\textsuperscript{9}.

Monitoring by the environment is a useful way of thinking about the emergence of the preferred set of states and about the process of decoherence in general. It can be shown that the interaction with the environment can be regarded as a continuous measurement of the pointer observable. As a consequence, the environment acquires a record of pointer observable. Its states become correlated with the preferred pointer states: Quantum state of the complete (system plus environment) object can be written as:

$$|\Psi> = \sum_i \alpha_i |\sigma_i> |\epsilon_i>,$$

where the states of the environment correlated to the eigenstates of the preferred observable become (to an excellent approximation) orthogonal (i.e., $<\epsilon_i|\epsilon_j> \propto \delta_{ij}$) as a result of the interaction with the system.

As the environment continuously acquires the record of the states \{|$\sigma_i>$\}, other states (linear superpositions of the preferred states) are unstable. Quantum coherence of superpositions of \{|$\sigma_i>$\} is lost: When a system is prepared in a state:

$$|\Phi> = \sum_i \alpha_i |\sigma_i>,$$

it will rapidly decay into a density matrix which is always diagonal in the same (preferred) basis:

$$|\Phi><\Phi| \rightarrow \rho \approx \sum_i |\alpha_i|^2 |\sigma_i><\sigma_i|.$$

Hence, the system behaves as if an effective superselection rule precluding existence of superpositions between the eigenstates of the preferred basis was in place.

Environment induced superselection rules effectively outlaw arbitrary superpositions. Thus, even though the superposition principle is valid in a closed quantum system, it is invalidated by decoherence for systems interacting with their environments. All of the macroscopic quantum systems we encounter in our everyday existence, as well as our own
memory and information processing hardware (e.g., neurons, etc) are macroscopic enough and sufficiently strongly coupled to the environment to be susceptible to decoherence, which will eliminate truly quantum superpositions on a very short timescale. This process is absolutely essential in the transition from quantum to classical in the context of quantum measurements (where the classical apparatus tends to be very macroscopic) although resolutions based on decoherence may not be easily palatable to everyone (i.e., see comments on decoherence in the April 1993 issue of Physics Today).

The timescale on which decoherence takes place can be estimated by solving a specific example: a one dimensional particle moving in a potential \( V(x) \) coupled through its position with a thermal environment – e.g. with a collection of harmonic oscillators at a temperature \( T \). Under the appropriate assumptions one can derive an equation for the reduced density matrix of the preferred particle. In the position representation it reads:\(^{18}\)

\[
\dot{\rho} = \begin{cases} 
\text{von Neumann eq.} & -\frac{i}{\hbar}[H_o, \rho] \\
\text{relaxation} & -\gamma(x-y)(\frac{\partial}{\partial x} - \frac{\partial}{\partial y})\rho \\
\text{decoherence} & -\frac{2m\gamma k_B T}{\hbar^2}(x-y)^2 \rho 
\end{cases} \\
\dot{p} = -\text{FORCE} = -\nabla V \\
\dot{p} = -\gamma p
\]

(mastereq)

Above, we have indicated the role of the three terms which constitute the master equation in the so–called high temperature limit – that is, in the case when the thermal excitations of the environment dominate the effect of the environment, and the effect of the vacuum fluctuations can be neglected.

Mathematically, classical limit is often associated with the size of Planck’s constant. In the limit \( \hbar \to 0 \) the very last term of the above equation becomes dominant. To understand its effect, let us write an explicit solution of (mastereq) approximating the right hand side by the last term only. In that case

\[ \rho(x, y, t) = \rho(x, y, 0) \exp(- (x-y)^2 D t/\hbar^2) \]

(rhot)

Above \( D = 2m\gamma k_B T \).

It is now apparent that the evolution under nothing but the decoherence term leaves the diagonal of the density matrix in the position representation essentially uneffected. By contrast, for \( x \neq y \) the density matrix will decay exponentially in a decoherence timescale:\(^{12}\)

\[ \tau_D = \gamma^{-1} \frac{\hbar^2}{D(x-y)^2} = \tau_R \left( \frac{\lambda dB}{\Delta x} \right)^2, \]

(dectime)
where \( \lambda_{dB} = (\hbar^2/2mk_BT)^{1/2} \) is the thermal de Broglie wavelength and \( \tau_R = \gamma^{-1} \) is the relaxation timescale.

Two remarks are in order: (i) The decoherence timescale \( \tau_D \) is much shorter than the relaxation timescale \( \tau_R \) for all macroscopic situations, as typical thermal de Broglie wavelengths of macroscopic bodies are many orders of magnitude smaller than macroscopic separations \( \Delta x \). (ii) The devastating effect of decoherence on superpositions of position can be traced back to the preferential monitoring of that observable \( (x) \) by the environment, which was coupled to the position of the system of interest. This also tends to be the case in general: Interaction potentials depend on position and, therefore, allow the environment to monitor \( x \). As a result of the action of the decoherence term, the vast majority of states which could in principle describe the system of interest would be, in practice, eliminated by the resulting environment - induced superselection. Only localized states will be able to survive. They will form a preferred basis. For (even though they will be in general still somewhat unstable under the joint action of the self–hamiltonian and the environment) they will be much more stable than their coherent superpositions. This can be gauged by estimating the timescale characterizing the rate of entropy production. For the preferred states this timescale will be relatively long, determined by the dynamics and relaxation. For example, in an underdamped harmonic oscillator the preferred states turn out to be the familiar coherent states: Oscillator dynamics rotates all of the states, which, in effect, translates spread in position into spread in momentum (and vice versa) every quarter period of the oscillation. As a result, coupling to position can be quite faithfully represented in the “rotating wave approximation” which makes the master equation symmetric in \( x \) and \( p \). Hence, coherent states will minimize entropy production. By contrast, for superpositions of coherent states entropy production will happen on a very much shorter decoherence timescale.

More general dynamics tends to deform states in the Hilbert space of the system. Chaotic dynamics is especially effective in this, as it reflects exponential stretching and squeezing of phase space distributions. Thus, a regular patch in the phase space will be relatively quickly (on a Lyapunov timescale) deformed into something which will be no longer regular. By the same token, localized preferred states will tend to be stretched into non–local superpositions. Thus, the form of a typical state on the diagonal of the density matrix of a chaotic system will be a matter of compromise between the chaotic dynamics and decoherence. We shall discuss the nature of this compromise in the next section.
3. DECOHERENCE VS. EXPONENTIAL INSTABILITY

Phase space provides a natural arena to study the consequences of the chaotic dynamics and its interplay with decoherence. Master equation (mastereq) can be translated into an equation for the Wigner distribution. The resulting equation consists of the Wigner transform of the commutator (which results in the so-called Moyal bracket) plus additional terms representing relaxation and decoherence:

\[ \dot{W} = \{H, W\}_MB + 2\gamma\partial_p p W + D\partial^2_{pp} W \]  

(wignereq)

where the first term on the right hand side denotes the Moyal bracket, which can be written in terms of the Poisson bracket as \( \{ , \}_MB = 2i\sin(\hbar\{ , \}_PB/2i)/\hbar \).

We will be interested in the regime in which the coupling to the environment is sufficiently weak so that the damping (represented by the second term in (wignereq)) is negligible. This is the so-called “reversible classical limit”\(^{12,15,13}\) which in integrable systems yields reversible classical trajectories but still eliminates non-local superpositions (this limit is achieved by letting \( \gamma \) approach zero but keeping \( D \) constant so that decoherence continues to be effective). In this limit, and in the case where the potential is analytic, equation (wignereq) can be rewritten as\(^{20}\):

\[ \dot{W} = \{H, W\}_PB + \sum_n \frac{\hbar^{2n}(-1)^n}{(2n+1)!2^{2n}} \partial_x^{(2n+1)} V \partial_p^{(2n+1)} W + D\partial^2_{pp} W. \]  

(wignereq2)

Thus, Liouville flow in the phase space (and, therefore, classical dynamics) is obtained from the basic quantum picture as long as the corrections appearing in (wignereq2) are negligible. However, in a chaotic system evolution of the Wigner function generated by the Poisson bracket takes it quickly into the regime where Poisson bracket alone does not suffice. This is because chaotic systems exhibit exponential sensitivity to initial conditions. Consequently, a phase space patch corresponding to a Wigner distribution will be exponentially stretched in the unstable directions corresponding to positive Lyapunov exponents. As the volume in phase space corresponding to \( W \) must be preserved, this will result in exponential shrinking in other directions. Consequently, derivatives of the Wigner function with respect to momentum (which enter into the correction term) will exponentially increase, so that after a time which is logarithmic in \( \hbar \) these initially small terms will become comparable to the Poisson bracket and Liouville dynamics will cease to be an accurate approximation. This argument leads, in fact, to a demonstration of equation (tchi), as the reader is encouraged to verify.
One can regard this breakdown of the Liouville dynamics as a consequence of the loss of validity of a classical formula for the force in terms of the gradient of the potential $V(x)$ (which is implemented in the Poisson bracket). As the Wigner function becomes more squeezed in momentum, by virtue of Heisenberg’s uncertainty principle it spreads in position, and it begins to coherently sample increasingly large regions of the phase space. This process results in the domination of the evolution operator by the quantum forces when the extent of the wavefunction in space becomes comparable with the scale of nonlinearity, which for the various terms in equation (wignereq2) is given by:

$$\chi_n = \left(\frac{\partial_x V}{\partial_x (2n+1)} V\right)^{1/2n}.$$  \hspace{1cm} (chin)

How can decoherence help reestablish the quantum - classical correspondence? Let us, for the moment, keep just the Poisson bracket and the diffusion term. Then, in the neighbourhood of any point, equation (wignereq2) can be easily expanded along the unstable ($\lambda^+_i > 0$) and stable ($\lambda^-_i < 0$) directions in phase space ($\sum_i (\lambda^-_i + \lambda^+_i) = 0$). Diffusion will have little influence on the evolution of $W$ along the unstable directions: After the possible initial (decoherence timescale) transient, $W$ will be stretched simply as a result of the dynamics, so that the gradients along these directions will tend to decay anyway, without assistance from diffusion. By contrast, squeezing which occurs along the contracting directions will tend to be opposed by the diffusion. This will lead to a steady state with the solution asymptotically approaching a Gaussian with a half–width given by the critical dispersion:

$$\sigma^2_{ci} = 2D_i/|\lambda^-_i| \hspace{1cm} (sigmacrit)$$

where $\lambda^-_i$ is the (negative) Lyapunov exponent along the stable direction and $D_i$ is the diffusion coefficient along the same direction. Below, we will assume that the diffusion is isotropic (as would be the case in the rotating wave approximation). Thus, after some time (and in the absence of folding – the other aspect of chaos which we will discuss below) the Wigner function will evolve into a multidimensional “hyper–pancake,” still stretching along the unstable directions but with its width limited from below in the stable directions by equation (sigmacrit).

At this stage, entropy will be approximated by the logarithm of the effective volume of the hyper–pancake. As its extent in the stable direction is fixed by the critical width (sigmacrit), its volume will tend to increase at a rate given by the positive exponents. Consequently,

$$\dot{H} \approx \sum_i \lambda^+_i. \hspace{1cm} (hdot)$$
This constant rate will set in after a time larger than the decoherence timescale (for smaller times the entropy production can be even more rapid) and after a time over which the initial Wigner distribution becomes squeezed by the dynamics to the dimension of order of the critical dispersion $\sigma_{c_i}$. Equation (hdot) will be valid untill the pancake fills in the available phase space and the system reaches (approximately) uniform distribution over the accessible part of the phase space, that is after a time defined by:

$$t_{eq} = (H_{eq}/H_0)/\dot{H},$$

(eqtime)

where $H_0$ is the initial entropy, and $H_{eq}$ is the entropy uniformized by the chaotic dynamics.

Astute reader will note that $H_{eq}$ above need not be a true equilibrium entropy with the temperature given by $T$. Rather, it will correspond to dynamical quasi–equilibrium – the approximately uniform distribution over this part of the phase space which is accessible to the chaotic system as a result of its dynamics.

The corresponding timescale will have a similar dependence on $\hbar$ as the timescale $t_\chi$ defined by Eq. (1). This is because entropy is approximately given by the logarithm of the volume of the phase space over which the probability distribution has spread in the units of Planck constant. Nevertheless, $t_\chi$ and $t_{eq}$ depend on rather different aspects of the initial and final state, and one can expect $t_\chi$ to be be typically a fraction of $t_{eq}$.

By contrast, in integrable systems stretching of the corresponding hyper–pancake in phase space will proceed only polynomially. Thus, even when it will get to the stage at which, in the contracting direction, diffusion will become important, stretching in the unstable direction will be only polynomial (rather than exponential). Consequently, the volume of the hyper–pancake will increase only as some power of time. Hence, the entropy will grow only logarithmically as the entropy production rate will fall as $\dot{H} \propto 1/t$: It will take exponentially long to approach dynamical quasi–equilibrium.

This difference in behavior between chaotic and integrable open quantum systems is striking and can be used as a defining feature of quantum chaos.

4. QUANTUM–CLASSICAL CORRESPONDENCE IN CHAOTIC SYSTEMS.

The failure of Ehrenfest theorem in chaotic systems is the consequence of the exponentially unstable Liouville flow which compresses Wigner function into an exponentially
narrowing pancake. As the momentum becomes progressively squeezed – which makes it less and less uncertain – the spatial extent of the coherent quantum wavefunction will exponentially increase until it eventually simultaneously samples much of the potential well. By then the force is no longer given by a gradient of the potential: The wavefunction is too non–local for such a formula. It would not be even clear where (within the spatial support of the wavefunction) one should compute such gradient. Instead, a more complicated formula, the Moyal bracket, is needed.

Decoherence limits the extent over which the wavefunction can remain coherent. This is because a finite minimal dispersion in momentum (sigmacrit) corresponds to quantum coherence over distances no longer than:

$$l = \frac{\hbar}{\sigma_c} = \frac{\hbar}{(2D/\lambda)^{1/2}}. \quad (lcrit)$$

Thus, when the scale (chin) on which nonlinearities in the potential are significant is small compared to the extent of the wavefunction

$$\chi \ll l \quad (chivsl)$$
decoherence will have essentially no effect. Evolution will remain purely quantum and will be generated by the full Moyal bracket.

By contrast, when the opposite is true, the evolution will never squeeze Wigner distribution function enough for the full Moyal bracket to be relevant. Poisson bracket will suffice to approximate the flow of probability in phase space. The inequality characterizing this case can be written in a manner reminiscent of the Heisenberg indeterminacy principle:

$$\hbar \ll \chi \sigma_c. \quad (ineqclass)$$

That is, as long as decoherence keeps the state vector from becoming too narrow in momentum, it will also prevent it from sampling the potential coherently over distances on which $V(x)$ is noticeably different from linear. Hence, local gradients will suffice in the evaluation of the forces – Poisson bracket is all that is required.

There is one more interesting regime where the chaotic motion is dynamically reversible (that is, $\dot{H} = 0$) even if the system satisfies inequality (ineqclass). This happens when the initial patch in phase space is large (volume much larger than the Planck volume – initial entropy larger than a single bit) and regular. Then the initial stage of the evolution will proceed reversibly, in accord with the Poisson bracket generated flow. Decoherence will
have little effect. This is because its influence will set in only as the dimension of the Wigner distribution in the contracting dimension will approach the critical dispersion $\sigma_c$:

In a simple example the entropy production will increase as:

$$\dot{H} = \lambda \frac{1}{\left(1 + \left(\frac{\sigma_p^2(0)}{\sigma_c^2} - 1\right) \exp(-2\lambda t)\right)}$$

So far, we have not taken into account (or, at least, not taken into account explicitly) the other major characteristic of chaos: In addition to exponential instability, chaotic systems “fold” the phase space distribution. While this problem may require further study, we believe that the fundamentals of folding are already implicit in the above discussion:

Folding will happen on the scale $\chi$ of nonlinearities in the potential (which will typically – but not always – coincide with the size of the system, as it is defined by the range of its classical trajectory). Hence, preventing the system from maintaining coherence over distances of the order of $\chi$ will also ascertain its classical behavior in course of folding. There will simply be no coherence left between the fragments of the wavepacket which will come into proximity as a result of folding, if they had to be separated by distances larger than $l$ in the course of the preceding evolution. Thus, folding will proceed as if the system was classical, but with a proviso: After sufficiently many folds the distribution function (which in the stable direction cannot shrink to less than $\sigma_c$) will simply fill in the available phase space. This will be achieved in the previously defined equilibrium timescale $t_{eq}$. These conclusions are consistent with the numerical studies of quantum maps corresponding to open quantum systems such as the “standard map” carried out by Graham and his coworkers.21

5. SUMMARY.

We have used the entropy production rate in a decohering quantum system to characterize the nature of its evolution. Classical unpredictability – the essence of dynamical chaos – was shown to beget quantum unpredictability, quantified by the rapid entropy production on the Lyapunov timescale. By contrast, dynamics of integrable systems leads to only gradual (polynomial) spread of the patch of the phase space corresponding to the state of the system. As a result, a much slower evolution towards dynamical quasi–equilibrium (and a relatively good predictability in spite of the coupling to the environment) charac-
terize quantum analogs of classically integrable systems. This distinction is conjectured to be a diagnostic of the dynamical nature of the system.

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Figure 1: The evolution of a “patch” in the phase space in a system with an exponential instability:

(a) The case when the system is isolated and only exponential stretching in the unstable direction as well as the corresponding shrinking in the complementary direction take place. The decrease of the dimension of the patch in momentum results (through the Heisenberg indeterminacy relation) in nonlocality, which leads to non–classical corrections to the expression for the force (resulting in the Moyal bracket).

(b) When the system is open, decoherence prevents the dispersion of momentum from shrinking to less than the critical dispersion $\sigma_c$. Critical dispersion characterizes the steady state set by the competition between the dynamics (which attempts to narrow the patch, as it was shown in Fig. 1a) and decoherence, which is associated with the diffusion operator (which attempts to spread the patch). When decoherence is sufficiently effective, the spatial extent of the coherence of the wavepacket (given by $l = h/\sigma_c$, $\text{lcrit}$) will be sufficiently small so that the harmonic approximation to the potential will be accurate. And in such linear regime Moyal bracket and Poisson bracket coincide. Therefore, classical dynamics can be recovered even for chaotic systems.