PHYSICAL REVIEW A VOLUME 30, NUMBER 1 JULY 1984

Ergodicity and mixing in quantum theory. I

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(Received 17 January 1984)

Quantum chaos is defined by the following property: Simple dynamical variables (position, momentum, etc.) are represented by pseudorandom matrices, when the Hamiltonian is diagonal. As a consequence, the expectation values of these variables tend to equilibrium values which are insensitive to the initial preparation, for nearly all preparations involving many energy levels. Moreover, the fluctuations around these equilibrium values are, on the average, very small.

I. INTRODUCTION

Classical ergodicity and mixing are well understood.[1,2] Their quantum analogs, however, have been controversial.[3] This may be due to the fact that classical chaos has many different facets[4] and some of these are without straightforward quantum analogs.

In this paper I propose a new approach, in which quantum chaos is defined intrinsically, in pure quantum language, without explicit reference to classical chaos. The hallmark of quantum chaos is that *simple dynamical variables (position, momentum,* etc.) *are represented by pseudorandom matrices when the Hamiltonian is diagonal.* This new approach emphasizes dynamical variables (rather than wave functions, as in most of the literature). Indeed, as Heisenberg's formulation of quantum theory is closer in its spirit to classical mechanics than Schrödinger's formulation, one should expect the former to be more suitable to discuss quantum chaos.

This approach is also radically different from the statistical theory of energy levels of random matrix Hamiltonians.[5–7] The latter is based on the assumption that the Hamiltonian is an utterly complicated function of positions and momenta. One then considers a random ensemble of such Hamiltonians, and one can investigate the statistical properties of their energy spectra. However, it is now well known that classical chaos can result from extremely simple Hamiltonians.[8,9] No more than two degrees of freedom are needed or, if the Hamiltonian is time dependent, a single degree of freedom is enough to have chaos.

The plan of this paper is as follows. In Sec. II it is argued that the proposed definition of quantum chaos is reasonable; that is, if a classical system is chaotic, its quantum analog is likely to be chaotic too. Here, the reader should not expect a rigorous proof. The argument is admittedly qualitative because the correspondence between quantum mechanics and classical mechanics is qualitative too, except in the limit $\hbar \to 0$. (A rigorous proof, valid in the limit $\hbar \to 0$, would probably be fraught with so many restrictions as to be practically useless.)

Section III discusses some questions about degeneracy and ergodicity. Section IV is devoted to mixing. It is shown that, in a chaotic system, the expectation values of "reasonable" dynamical variables tend to equilibrium values which are insensitive to the details of the initial-state preparation, for nearly all preparations involving *many* energy levels. Here, the reader should note that "many" is not "infinitely many." No thermodynamic limit is considered in this paper. There may be fluctuations around the equilibrium value but these are, on the average, very small. In paper II[10] the above ideas will be illustrated by two numerical examples, one with the Hénon-Heiles model and one with a pair of nonlinearly coupled rotators.

II. CHAOS

The purpose of this section is to explain the motivation for the proposed definition of quantum chaos. In essence it says that any "reasonable" dynamical variable has many "random" matrix elements in the energy representation. It cannot be a sparse matrix with mostly zeros and only a few large elements. The argument can therefore be divided in two steps: (i) Any reasonably simple variable (position, momentum, etc.) indeed has that property and (ii) conversely, any numerically "simple" matrix represents an utterly complicated (experimentally inaccessible) dynamical variable.

Before I show that the above properties are indeed likely to hold for generic classically chaotic systems having quantum analogs, a more precise meaning must be given to the terms reasonable and random. Reasonable operators (also called "classical operators") have been rigorously defined by Yaffe[11] and include, e.g., polynomials in p and q with no explicit $\hbar$ dependence. In particular, a quantum system has a classical analog if the Hamiltonian is a classical operator. Formally, one ought to consider a *sequence of quantum theories* endowed with different values of $\hbar$ and examine whether the limit $\hbar \to 0$ coincides with classical mechanics. In general, quantum theory does *not* reduce to classical mechanics for arbitrary states, only for those having $\Delta p\, \Delta q \to 0$ as $\hbar \to 0$ (for example, coherent states). In quantum field theory a reasonable operator is essentially the same as a "quasilocal operator."[12] For our purpose it will be enough to define a reasonable operator $A = f(p,q,\hbar)$ by the property that the "classical" $A = f(p,q,0)$ is a nonpathological function of p and q.

Familiar *nonclassical* operators are parity, and modular variables[13] such as L_z (mod$3\hbar$) which is a constant of motion of the Hénon-Heiles system.[14] These nonclassical operators will not, in general, have random matrix elements in the energy representation.

Next, I will explain what is meant by a random, or rather a *pseudorandom* matrix. It is best to do this by means of an example. Consider the three angular momentum matrices L_x, L_y, and L_z in their standard textbook representation (with L_z diagonal). These matrices are sparse: Most of their elements are zeros. Now consider the three matrices $\vec{L}\,' = U\vec{L}U^{\dagger}$, where U is a random unitary matrix. The matrices $\vec{L}\,'$ are not sparse: All their elements may have roughly the same order of magnitude (an explicit example is given in paper II). They may thus appear random to the untrained eye. Yet, they are not random at all. The eigenvalues $(l, l-1, \ldots, -l)$ are invariant and the commutation relations $[L_x', L_y'] = i\hbar L_z'$ remain valid under any unitary transformation. In other words, the pseudorandom matrix elements are subject to many *correlations.* However, these correlations are highly "nonlocal" because they involve sums over the *full range of indices,* e.g., $\sum_m (L_x')_{mm} = 0$. If we can examine only a submatrix of L_x', it does appear random.

It is now possible to explain why reasonable dynamical variables are represented by random matrices when the Hamiltonian is diagonalized. This property readily follows from Percival's conjecture[15] that a nonintegrable Hamiltonian has "disordered" eigenfunctions, such that any elementary operator (p, q, etc.) has matrix elements of the same order of magnitude between any two of these eigenfunctions (because there are no selection rules). Although Percival's conjecture is too vague to be proved formally, it is by now well established as a qualitative guideline. It is not only supported by many more-or-less rigorous theoretical arguments,[16–19] but also by a large amount of empirical evidence in computer simulations of chaotic systems.[20–24] The situation has been summarized by Pechukas.[25] "All eigenfunctions of roughly the same energy look roughly the same: Each is spread over the entire classically allowed region of configuration space appropriate to its energy, with a coarse-grained probability density that agrees well at each point of space with the classical microcanonical density at that energy."

Nevertheless, recent investigations have conclusively shown that classical chaos does *not* necessarily imply quantum chaos (at least for finite values of $\hbar$).[26–28] Quantum chaos is usually more remote than classical chaos because of the existence of "tori remnants" in the chaotic part of the classical phase space. As long as the missing parts of these "vague tori" are small compared to $2\pi\hbar$, the quantum system behaves as if it were regular, with approximately valid selection rules.[29,30]

Moreover, there are classical systems such as the Hénon-Heiles oscillator[14] which have mostly regular orbits in some regions of phase space and mostly chaotic orbits in other regions. In that case we expect that reasonable operators will be represented by matrices which are sparse for some range of their indices and pseudorandom for a different range of the indices. A numerical example is given in paper II.

Let us consider for simplicity the purely chaotic case. If the position and momentum operators are represented by pseudorandom matrices, the same is likely to hold, by the rules of matrix multiplication, for any operator which is a polynomial in p and q, or can be defined by any other *finite* algorithm. (An obvious exception is the Hamiltonian, which is diagonal by construction.)

On the other hand, if we wish to construct a dynamical variable represented by a numerically simple nondiagonal matrix (mostly zeros and just a few nonvanishing elements), this can only be done through an *infinite* sequence of operations involving p and q. Although such a variable "exists" in some abstract mathematical sense, it would have enormous algorithmic complexity[31] and be inaccessible to experimental physicists. Indeed, not every self-adjoint operator corresponds to an actually measurable property.[32]

In summary, I propose to *define* "quantum chaos" by the property that all dynamical variables having a simple physical meaning are represented by pseudorandom matrices when the Hamiltonian is diagonal (with the obvious exception of the Hamiltonian itself and functions thereof). Some consequences of this definition will be discussed in Secs. III and IV.

III. ERGODICITY AND DEGENERACY

In this section I first review the traditional definitions of quantum ergodicity and then I propose a new approach based on the above definition of quantum chaos. The status of quantum ergodicity is somewhat confused (one would be tempted to say chaotic). The original definition, due to von Neumann[33] and extended by other authors,[34–37] was criticized for a variety of reasons. It was claimed[38] that "quantum mechanical systems do not have ergodic character" because the energy spectrum of a system with several degrees of freedom is degenerate. Contrariwise, some authors[39,40] asserted that von Neumann's ergodicity was a trivial consequence of the averaging over "macro-observers" and had nothing to do with quantum dynamics.

The root of the difficulty is the following. Classical ergodicity has a precise meaning: The time average of a dynamical variable is the same as its phase-space average. The latter is computed by dividing phase space into small cells and the problem is how often a given classical orbit visits each cell. Unfortunately, these classical small cells have no quantum equivalent. The customary approach, initiated by von Neumann, is to consider M-dimensional subspaces in an N-dimensional "energy shell" spanned by N consecutive eigenvectors of the Hamiltonian (with $N \gg M \gg 1$). This seems to assume, tacitly, that subspaces of low dimensionality are the analog of small phase-space regions, which is certainly wrong.[41] In particular, Wigner's distributions[42] in two neighboring regions of phase space (of size much larger than $\hbar$) do *not* correspond to neighboring quantum states, but to *orthogonal* states. In general, it appears that the emphasis on *states* (or wave functions) is not fruitful and is the cause of all the above confusion. As I already explained, *dynamical variables* (and their expectation values) are a concept much closer to classical mechanics and also to experimental physics.

Another difficulty in matching classical and quantum ergodicities is that the latter depends on whether the Hamiltonian has a degenerate spectrum. At first sight one would naively expect that a classically nonintegrable system, having no other isolating constant of the motion than the Hamiltonian itself, should have a nondegenerate energy spectrum. The real situation is far more complex.

First, there are systems which are only partly integrable, such as the hydrogen atom in a uniform magnetic field (there are three degrees of freedom and only two constants of motion).[43] Moreover, there are in quantum theory discrete symmetries with no classical analog, such as parity, or the C_{3v} symmetry of the Hénon-Heiles system.[14] These symmetries correspond to nonclassical constants of motion.[13] In particular, since the C_{3v} group is not Abelian, it must lead to a degeneracy of the quantized Hénon-Heiles energy spectrum. These discrete symmetries of the Hamiltonian obviously prevent quantum ergodicity (in the usual sense of this word) as no transition is possible between states of different symmetry classes.[44] Thus, a quantum system may *not* be ergodic although its classical analog is.

And *vice versa,* there may be classically integrable systems which are not integrable in quantum theory because of factor ordering problems.[45,46] To further add to the confusion, semiclassical quantization (i.e., the Einstein-Brillouin-Keller method) typically disagrees with quantum mechanics. In general, it predicts higher degeneracy than is actually observed.[47,48]

At this point it is advisable to recall why classical ergodicity is a useful property. Its importance resides in the fact that, in an ergodic system *the time average of a dynamical variable depends only on the total energy and not on the other details of the initial state.* Thus, the real question is whether a similar property holds in quantum theory.

The quantum expectation value of a dynamical variable $A(t)$ is

$$\langle A(t)\rangle_Q=\sum_{E'}\sum_{E''}\rho_{E'E''}A_{E''E'}e^{i(E''-E')t}\ , \tag{1}$$

where $\rho_{E'E''}$ is the density matrix in the energy representation. (The system is assumed bounded, so that its spectrum is discrete, and $\hbar=1$, as usual.) If the energy spectrum is not degenerate, the time average of (1) is

$$\langle\langle A(t)\rangle_Q\rangle_T=\sum_{E}\rho_{EE}A_{EE}\ , \tag{2}$$

which is independent of the initial phases (appearing in the off-diagonal elements of ρ). For a degenerate system the formula is slightly more complicated and involves off-diagonal elements of ρ.[49] I shall henceforth assume that the system is nondegenerate, for simplicity, and later point out where degeneracy makes an essential difference.

Consider the right-hand side (rhs) of Eq. (2). Assume that the ρ matrix has nonvanishing elements in a finite energy range ΔE. For example, if the system has been prepared by a macroscopic apparatus at temperature T, we must have $\Delta E \gtrsim kT$. Assume that there are many energy levels in the range ΔE. (If there are only a few levels, the system will be quasiperiodic with a relatively short recurrence time. However, if there are many incommensurate levels, the recurrence time is so long[50] that it can be ignored.)

The distribution of these energy levels is very different for regular and chaotic systems because it is related to the properties of closed classical orbits. Gutzwiller[51] was the first to predict that the density of quantum states $D(E)$ corresponding to stable *versus* unstable orbits would be qualitatively different. Balian and Bloch[52] showed that, on scales large compared to the mean level spacing, $D(E)$ is a smooth oscillatory function, well approximated by the contributions of short closed paths. They gave explicit examples of density oscillations for the wave equation in a finite enclosure. Berry and Tabor[53] discussed the *regular* spectrum with full generality and confirmed that $D(E)$ oscillates with a "wavelength" of order $\hbar\omega_c$. (Here ω_c denotes a typical frequency of a closed periodic orbit.) Finally, Berry[54] showed that the amplitudes of the oscillations in $D(E)$, on scales $\sim\hbar\omega_c$, are smaller for classically chaotic systems than for classically regular ones. [In addition to these large scale oscillations of $D(E)$, there is also a repulsion of *individual* levels in chaotic systems[55–57] which, however, has no direct effect on the time scale considered here.]

The above discussion describes the properties of the ρ_{EE} term in the rhs of (2). The A_{EE} term, too, behaves very differently for regular and chaotic systems. Regular systems have selection rules such that most A_{EE} vanish and only a few are large. Chaotic systems have (by definition) pseudorandom A_{EE}. [Of course, a chaotic system may also have selection rules due to nonclassical symmetries, such as parity: If $H(x)=H(-x)$, then $x_{EE}=0$.]

Let us therefore consider the rhs of (2) in the chaotic case for a narrow but finite range ΔE around some mean energy $\bar{E}=\sum_E E\rho_{EE}$. (Here "narrow" means that the properties of the classical phase space are approximately the same in the range $\bar{E}\pm\Delta E$.) In that narrow range there are *many* pseudorandom A_{EE}, which are statistically independent of the ρ_{EE}, for *nearly* every conceivable preparation of the system (see below). These A_{EE} are so numerous that their *average* does not appreciably depend on ΔE and thus can be simply denoted by $\bar{A}(\bar{E})$. As $\sum_E\rho_{EE}=1$, we obtain

$$\langle\langle A(t)\rangle_Q\rangle_T=\bar{A}(\bar{E})\ . \tag{3}$$

Equation (3) defines quantum ergodicity.

On the other hand, for a regular system A_{EE} is sparse and $D(E)$ is clumpy, so that the approximations leading to Eq. (3) would be valid only for a very *broad* range ΔE, so broad that the properties of the classical phase space are qualitatively different for $\bar{E}\pm\Delta E$. Therefore Eq. (3) is generally not valid for a regular system and a reasonable ΔE.

Is a chaotic system (as defined in Sec. II) necessarily ergodic? There may be several reasons that it is not. One is related to the phrase "for *nearly* every conceivable preparation of the system" (see above). It may indeed be very difficult, but it is not theoretically impossible, to prepare a $\rho_{E'E''}$ matrix which statistically correlated to a pseudorandom $A_{E'E''}$ matrix. This is analogous to the possibility of having, in a classically chaotic system, closed periodic orbits which are not ergodic. Although these unstable periodic orbits are dense (for most Hamiltonian systems),[58] they form a set of measure zero. We can therefore safely ignore this difficulty.

Another difficulty is more serious and is related to degeneracy. If energy levels need two labels, E and α, for instance, Eq. (2) becomes

$$\langle\langle A(t)\rangle_Q\rangle_T=\sum_{E,\alpha,\beta}\rho_{E\alpha,E\beta}A_{E\beta,E\alpha}\,. \tag{2'}$$

We can still define, as usual, $\bar{E}=\sum_{E,\alpha}E\rho_{E\alpha,E\alpha}$. However, it is now impossible to derive (3) from (2′), unless $\rho_{E\alpha,E\beta}=\rho'_{EE}\delta_{\alpha\beta}$ (which is true for thermodynamic equilibrium, but not in general) or

$$\sum_{\substack{\alpha,\beta\\ \alpha\neq\beta}}A_{E\beta,E\alpha}=0\,,$$

or some similarly restrictive condition holds. This is not surprising. As already mentioned, a Hamiltonian endowed with a symmetry group generates a nonergodic evolution because no transitions are possible between states belonging to different symmetry classes.[44]

Still another difficulty appears for bistable or, more generally, multistable systems, such as multiple potential wells. In that case there may be, in the same narrow energy range ΔE, wave functions localized in different wells with very little overlap. Then, a reasonable (i.e., quasilocal) operator has vanishingly small matrix elements connecting these different sets of wave functions. It is therefore *not* represented by a random matrix (because many elements vanish), but it is reducible to a block-diagonal form, each block being a random submatrix, with zero elements outside the blocks. The rhs of Eq. (2) can then be written as a sum of contributions from the different blocks, corresponding to the various wells. We have, instead of Eq. (3),

$$\langle\langle A(t)\rangle_Q\rangle_T=\sum_j w_j\bar{A}_j(\bar{E})\,, \tag{4}$$

where $w_j=\sum_j\rho_{EE}$ (the sum being taken over all the energy levels localized in the jth well) and a similar definition holds for $\bar{A}_j(\bar{E})$. The time average of $\langle A(t)\rangle_Q$ thus depends not only on the total energy $\bar{E}$, but also on the probabilities w_j of finding the system in the various wells. Note that these probabilities are constant, because there can be no tunneling, unless the energy levels are degenerate.

IV. MIXING

Mixing is a stronger property than ergodicity. It is closely related to irreversibility. It requires that $\langle A(t)\rangle_Q$ itself tend to a constant—an equilibrium value—for $t\to\infty$. It has been claimed[49] that "because of the discreteness of the energy, this concept does not play a role in the quantum theory of finite systems." Indeed, any multiply periodic function such as in Eq. (1) must have recurrences.[59] (A similar result also holds for Hamiltonians which are time periodic[60] rather than simply time independent.) However, unless the number of energy (or quasienergy[60]) levels is extremely small, the time required for these recurrences is so huge that it is physically uninteresting.[50]

I shall therefore consider a less stringent requirement (which may be called "weak mixing") which is that the *fluctuations* of $\langle A(t)\rangle_Q$ around its equilibrium value $\bar{A}(\bar{E})$ are typically small. This does not preclude rare large fluctuations or even a recurrence of the initial state after a huge time. In other words, I do not seek the limit $t\to\infty$ which does not exist for a finite system, but rather consider "most times."

It is not difficult to prove that the fluctuations of a chaotic and nondegenerate system are typically small. The time average of their square is

$$F^2=\langle[\langle A(t)\rangle_Q]^2\rangle_T-[\langle\langle A(t)\rangle_Q\rangle_T]^2\,. \tag{5}$$

The first term contains expressions such as $\exp[i(E_1-E_2+E_3-E_4)t]$. Barring an accidental degeneracy of energy-level differences, these expressions have a nonvanishing time average only if $E_1=E_2$ and $E_3=E_4$ or $E_1=E_4$ and $E_2=E_3$. Collecting all the nonvanishing terms, we obtain

$$F^2=\sum_{E'}\sum_{E''}|\rho_{E'E''}|^2|A_{E'E''}|^2-\sum_E|\rho_{EE}A_{EE}|^2\,. \tag{6}$$

It is convenient to omit the last term in (6) and replace the equal sign by $\leq$.

At this point, I again introduce the assumptions that were used to prove ergodicity. Namely, the density matrix ρ representing the state preparation has nonvanishing elements in some narrow energy range ΔE containing a large number N of energy levels and, moreover, *nearly every* conceivable state preparation gives a ρ matrix which is *statistically independent* of the A matrix. It then follows from (6) that

$$F^2\leq\bar{A}^2(\bar{E})\sum_{E'}\sum_{E''}|\rho_{E'E''}|^2\,, \tag{7}$$

where $\bar{A}^2(\bar{E})$ is the average value of $|A_{E'E''}|^2$ in the energy range ΔE.

Moreover,

$$N^{-1}\leq\sum_{E'}\sum_{E''}|\rho_{E'E''}|^2=\mathrm{Tr}(\rho^2)\leq 1\,, \tag{8}$$

the limiting values corresponding to an equal weight mixture and a pure state, respectively. A typical preparation must be close to the lower limit, as it is quite difficult to prepare nonstationary states with precise phase relations between many energy levels. (This is certainly true if $\Delta E\simeq kT$, i.e., when the system is prepared by a macroscopic apparatus working at a temperature T.) Therefore the rms fluctuation

$$F\lesssim[\bar{A}^2(\bar{E})/N]^{1/2}\,, \tag{9}$$

is small, since N is large.

In summary, the equilibrium value $\bar{A}(\bar{E})$ is insensitive to the initial preparation (except for its mean energy) and the rms fluctuations around this equilibrium value are small. After a finite time the system does not "remember" how it was prepared and the evolution is said to be "irreversible." A numerical example, involving the Hénon-Heiles system, will be presented in paper II.[10]

ACKNOWLEDGMENTS

I am grateful for the hospitality of Nordisk Institut for Teoretisk Atomfysik NORDITA and that of Boston University where this work was brought to completion.

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