Chaotic evolution in quantum mechanics

Asher Peres*
Department of Physics, Technion—Israel Institute of Technology, 32 000 Haifa, Israel
(Received 10 August 1995)

A quantum system is described, whose wave function has a complexity that increases exponentially with time. Namely, for any fixed orthonormal basis, the number of components required for an accurate representation of the wave function increases exponentially. [S1063-651X(96)01905-8]

PACS number(s): 05.45.+b

This article describes a quantum system whose representation becomes increasingly complex with the passage of time. This behavior, which is well known as a generic property of *classical* Hamiltonian systems, is commonly called ''chaos.'' For example, an initially smooth Liouville density becomes more and more convoluted as time passes and it may form intricate shapes with exceedingly thin and long protuberances. However, quantum wave functions usually have a milder behavior [1]. In particular, quantum systems with discrete spectra can be represented, with arbitrary accuracy, by a *finite* number of eigenfunctions that are periodic in time. Their wave function thus is almost periodic. Its *computational complexity* [2, 3] does not increase as time passes. (Some authors use other criteria for complexity, such as the visual appearance of wave functions, but these seem rather subjective.)

There is nonetheless a simple way of generating a quantum chaos that closely parallels *any* type of classical chaos [4]. Consider an autonomous dynamical system obeying the equations of motion

$$dx^k/dt = V^k(x^1, \ldots, x^N), \quad k = 1, \ldots, N. \tag{1}$$

If $N \geqslant 3$, such a system may be chaotic. Irrespective of its physical nature, it is always formally possible to introduce a Hamiltonian

$$H = \sum_k V^k(x^1, \ldots, x^N) p_k, \tag{2}$$

where the p_k are new variables, defined to be canonically conjugate to the x^k. This Hamiltonian obviously gives Eq. (1) as the law of motion. (Note that the Lagrangian $L \equiv \Sigma p_k \dot{x}^k - H$ is numerically equal to zero. This is a highly constrained canonical system.)

Quantization may then proceed as usual by the introduction of a wave function $\psi(x^1, \ldots, x^N)$ and the substitution $p_k \to -i\hbar\,\partial/\partial x^k$. We then still have Eq. (1) as the Heisenberg equation of motion for the operators x^k and since the latter commute (and therefore can be simultaneously diagonalized) any chaos in the solution of the classical equations (1) will be reflected as chaos in the time evolution of the expectation values $\langle x^k(t) \rangle$. We thus see that there is no formal incompatibility between quantum theory and chaos. A simple example, the configurational cat map [5], was analyzed by Weigert. This quantization technique was also discussed by Berry [6].

In this article I present a detailed description of a quantum system whose wave function becomes increasingly complex with time, just as a Liouville density would do in classical mechanics. The long-range evolution of the wave function is effectively unpredictable with finite computing resources. This is a genuine example of quantum chaos. I have no pretense that the abstract model discussed here represents, even approximately, a real physical object. However, it gives a quantitative illustration to the fact that, contrary to some claims, quantum mechanics is compatible with the existence of chaos.

Such a chaotic quantum system can be constructed for any classical area-preserving map. As a concrete example I shall choose a map consisting of alternating twists and turns of a unit sphere. That map has a quantum version, called ''kicked top'' [7], with a discrete, finite-dimensional quasienergy spectrum. Therefore, unlike the classical map, the quantum kicked top is not truly chaotic. However, a classical dynamical system may have several, different quantum versions. Another quantization of the same twist and turn (TT) map is presented here, which is just as chaotic as the original classical map.

The latter is defined as follows. Consider the unit sphere $x^2 + y^2 + z^2 = 1$. Each step of the TT map consists of a twist by an angle a around the z axis (namely, every xy plane turns by an angle az), followed by a 90° rigid rotation around the y axis. The result is

$$\begin{aligned} x' &= z, \\ y' &= x\sin(az) + y\cos(az), \\ z' &= -x\cos(az) + y\sin(az). \end{aligned} \tag{3}$$

This map is obviously area preserving. For low values of a, most classical orbits are regular (that is, they are quasiperiodic). As a increases, so does the fraction of chaotic orbits, until for $a = 3$ most of the sphere is visited by a single chaotic orbit (all numerical calculations below refer to the case $a = 3$).

The kicked top [7] is a mechanical system (classical or quantal) that mimics the above geometrical map. In the classical case, the top has a three-dimensional generalized phase

*Electronic address: peres@photon.technion.ac.il

space [8], with canonical variables J_x, J_y, and J_z satisfying Poisson brackets $\{J_x, J_y\} = J_z$ and cyclic permutations. The mapping

$$J_x' = J_z,$$

$$J_y' = J_x \sin(aJ_z/J) + J_y \cos(aJ_z/J), \tag{4}$$

$$J_z' = -J_x \cos(aJ_z/J) + J_y \sin(aJ_z/J)$$

is a canonical transformation [9] that leaves J^2 invariant. The classical values of J_x/J, J_y/J, and J_z/J lie on a unit sphere and therefore they transform just as x, y, and z in Eq. (3).

A natural way of quantizing these equations is to replace the classical variables J_k by the corresponding quantum operators. Equation (4) then becomes a quantum map, generated by the *unitary* transformation

$$U = \exp(-i\pi J_y/2\hbar)\exp(-iaJ_z^2/2J\hbar). \tag{5}$$

For any eigenstate of J, this U is a matrix of order $(2j+1)$, with a discrete spectrum. The evolution is multiply periodic and there is no chaos analogous to that of the classical map: computing the wave function for long times is not more difficult than for short times. (There still is hypersensitivity to small perturbations [10], but this is not ''chaos'' in the classical sense.)

We can also consider quantum systems that are not restricted to a particular value of j. Their Hilbert space is spanned by the spherical harmonics $Y_j^m(\theta,\phi)$, with angles θ and ϕ related to the Cartesian coordinates in Eq. (3) in the usual way: $x = \sin\theta\cos\phi$, etc. The unitary evolution is still generated by Eq. (5), where it is now understood that the various J_k have to be written as block-diagonal matrices, with blocks of order $2j+1$. In that case, it is also possible to write the wave function as

$$\psi(\theta,\phi) = \sum_{j,m} C_{jm} Y_j^m(\theta,\phi), \tag{6}$$

but its components with different j are never mixed by the U matrix. They evolve independently of each other. There still is no chaos: the asymptotic cost of computing the final state does not increase with the number of steps. We thus see that the quantum kicked top is not a faithful replica of the classical TT map. The reason for this failure of the correspondence principle is explained below and an alternative quantization method will be proposed.

Consider the Hamiltonian that generates the unitary map (5):

$$H = aJ_z^2/2J + (\pi J_y/2)\sum_n \delta(t-n), \tag{7}$$

where the unit of time is the duration of one step. In this Hamiltonian, the twist is continuous and the rotation proceeds by kicks (the opposite choice is also possible). If ψ is represented by a set of C_{jm} coefficients as in Eq. (6), the J_k in (7) are block diagonal, as explained above. On the other hand, we may as well use the ''coordinate basis'' and directly write $\psi(\theta,\phi)$ without expanding into spherical harmonics, which is closer to the spirit of the classical TT map. We then have $J_z = -i\hbar\partial/\partial\phi$, and more complicated differential operators for J_x and J_y [11]. In particular,

$$J = -i\hbar\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]^{1/2}. \tag{8}$$

When we were in a finite-dimensional Hilbert space, it was natural (indeed unavoidable) to write the twist generator as $J_z^2/2J$. However, for arbitrary $\psi(\theta,\phi)$, a more natural expression for the twist generator is $J_z\cos\theta$. Let us therefore replace (7) by

$$H = aJ_z\cos\theta + (\pi J_y/2)\sum_n \delta(t-n). \tag{9}$$

This is a Hermitian operator that does not commute with J^2, so that J^2 is not conserved. (In other words, $J_z\cos\theta$ has nonvanishing matrix elements between Y_j^m with different j and cannot be written solely in terms of the J_k matrices.) Instead of (5) we now have

$$U = \exp(-i\pi J_y/2\hbar)\exp(-iaJ_z\cos\theta/\hbar). \tag{10}$$

The crucial difference is that the spectra of the new H and U include *continuous* parts and therefore permit the existence of true chaos. This can be shown as follows. Returning to the classical TT map (3), let us consider, instead of individual points, a mass density $\rho(\theta,\phi)$ spread on the unit sphere. We may even consider *complex* densities, if we wish. Let us further assume that the infinitesimal mass $\rho(\theta,\phi)d\Omega$, attached to the area element $d\Omega = \sin\theta d\theta d\phi$, is conserved by the TT map. It thus behaves as an incompressible fluid, or as a Liouville density would do while moving in phase space.

As the map is area preserving, namely, $d\Omega' = d\Omega$, we have, at each step,

$$\rho'(\theta,'\phi') = \rho(\theta,\phi). \tag{11}$$

This implies that the map is *unitary*: for any two densities ρ_1 and ρ_2,

$$\int \rho_1'(\theta',\phi')^* \rho_2'(\theta',\phi') d\Omega' = \int \rho_1(\theta,\phi)^* \rho_2(\theta,\phi) d\Omega. \tag{12}$$

Such a unitarity property was proved long ago by Koopman [12] for Liouville densities in phase space. Koopman's theorem applies only to the subset of Liouville densities that are square integrable. There also are, in classical mechanics, legitimate Liouville densities that are not square integrable. For these, Eq. (12) has no meaning; it is impossible to use Hilbert space methods that mimic quantum mechanics, and very little is known.

On the other hand, there is a large body of knowledge on the ergodicity and mixing properties of square-integrable Liouville functions [13]. In the generic nonintegrable case, the Liouvillian has a *continuous* spectrum, in which an infinite number of discrete lines may be embedded. If the dynamical system has a finite measure, the unitary operator U has at least one eigenvalue equal to 1, corresponding to equilibrium. Moreover, it can be proved [13] that, if the system is

ergodic but not mixing, that eigenvalue is nondegenerate and all the other eigenvalues of U form a subgroup of the circle group. On the other hand, for a mixing system, which also has a single nondegenerate eigenvalue 1, the rest of the spectrum is absolutely continuous. A generic dynamical system may have some regions of phase space that are subject to mixing, others that are only ergodic, and still others that are not even ergodic. Such a system is called ''decomposable'' [14]. In that case, the spectrum of U is continuous, with an infinite number of discrete lines embedded in it. In particular, the eigenvalue 1 and possibly others are degenerate.

Now, it is easily seen that the quantum wave function $\psi(\theta,\phi)$ behaves, under the unitary transformation U in Eq. (10), exactly as the fictitious incompressible mass density described above. This is obvious for the rotation operator $\exp(-i\pi J_y/2\hbar)$, which performs a rigid rotation of ψ around the y axis. For the twist $\exp(-iaJ_z\cos\theta/\hbar)$ we have

$$\psi(\theta,\phi)\rightarrow\psi'(\theta,\phi)=\psi(\theta,\phi-a\cos\theta). \tag{13}$$

That is, the wave function ψ moves on the surface of the unit sphere exactly as the classical points did and it remains normalized by virtue of the unitarity of the mapping. The essential difference between this new quantum system and the former kicked top is that the new Hamiltonian (which formally behaves as a classical Liouville operator) has a partly continuous spectrum. Therefore the evolution of $\psi(\theta,\phi)$ cannot be represented, even approximately, by a finite number of terms.

Let us examine this evolution more closely. The rotational part of U is represented, in the Y_j^m basis, by the familiar orthogonal matrix $U^{(j)}_{mm'}$, namely, a block-diagonal matrix with blocks of size $(2j+1)$ [15, 16]. In the same basis, the twist (13) is also represented by a unitary transformation [17]

$$C_{jm}\rightarrow C'_{jm}=\sum_l U^{(m)}_{jl}C_{lm}, \tag{14}$$

where

$$U^{(m)}_{jl}=\int Y_j^{m*}(\theta,\phi)Y_l^m(\theta,\phi)e^{-ima\cos\theta}d\Omega \tag{15}$$

is a band matrix. This transformation leaves m invariant, but introduces all the j with $j>|m|$ (with exponentially small coefficients for large j).

It is now possible to give a quantitative measure for the complexity of the wave function. Its information entropy [18]

$$S=-\sum_{j,m}|C_{jm}|^2\ln|C_{jm}|^2 \tag{16}$$

has the intuitive meaning that e^S roughly indicates the number of basis vectors that are appreciably involved in the expansion of ψ into spherical harmonics. This ''entropy'' of course depends of the choice of the basis (namely, spherical harmonics). However, it can be shown [17] that when S becomes large, its value is asymptotically independent of the choice of the basis, provided that the transformation between different bases is given by a band matrix (the latter property holds for any two bases whose definition is not algorithmically complex [19]).

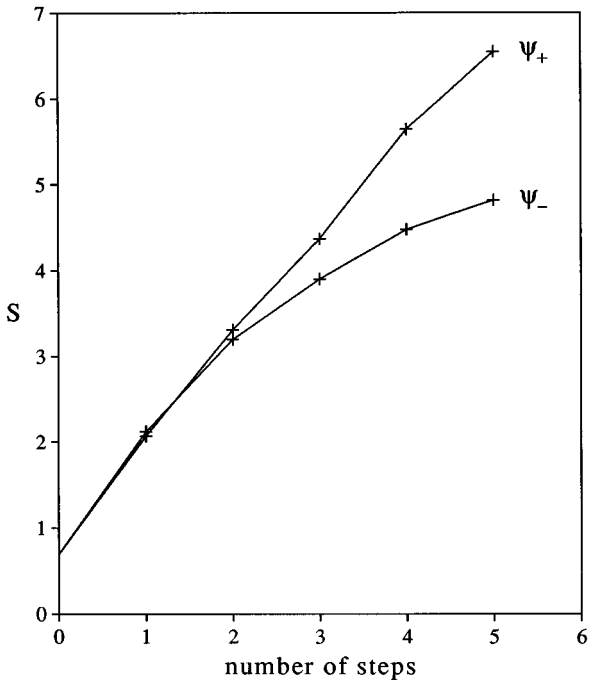

FIG. 1. Growth of S for the two initial states in Eq. (17).

Let us illustrate the above considerations by a numerical example. A plot of S versus the number of steps is shown in Fig. 1 for $a=3$, and for two initial states $\psi_\pm$ with

$$C_{11}=\pm C_{1,-1}=1/\sqrt{2}, \tag{17}$$

respectively, and all other $C_{lm}=0$. It is seen that S increases roughly linearly, so that, as the wave function evolves and becomes more and more complicated, the effective number of components needed for representing it increases about exponentially with time. The small negative second derivative seen in the graphs of Fig. 1 is due to the presence of small regular (nonchaotic) domains in phase space [7, 10], whose contributions to the growth of S is logarithmic rather than linear. (The calculation of the last step in Fig. 1 involved all the matrices with j,l,m up to 500. The next step would have exceeded the capacity of my workstation or entailed a severe loss of accuracy.)

Finally, it should be pointed out that the properties of the above model are generic. Any classical, bounded system for which a Liouville equation can be written can be quantized in this way (this is not, of course, the standard canonical quantization, since phase space is treated as if it were a configuration space and the number of dimensions is doubled). If the classical system is chaotic, so is the corresponding quantum system.

Some of the ideas presented here originated during a visit to the International Center of Theoretical Physics, Trieste, whose hospitality is gratefully acknowledged. I had interesting discussions with Felix Izrailev and Dima Shepelyansky. This work was supported by the Gerard Swope Fund and the Fund for Encouragement of Research.

[1] H. J. Korsch and M. V. Berry, Physica D **3**, 627 (1981).
[2] C. H. Bennett, in *Emerging Syntheses in Science*, edited by D. Pines (Addison-Wesley, Reading, MA, 1987), pp. 215–231.
[3] G. Brassard and P. Bratley, *Fundamentals of Algorithmics* (Prentice-Hall, Englewood Cliffs, NJ, 1995), Chap. 12.
[4] B. V. Chirikov, F. M. Izrailev, and D. L. Shepelyanski, Physica D **33**, 77 (1988).
[5] S. Weigert, Z. Phys. B **80**, 3 (1990); Phys. Rev. A **48**, 1780 (1993).
[6] M. V. Berry, in *New Trends in Nuclear Collective Dynamics*, edited by Y. Abe, H. Horiuchi, and K. Matsuyanasi, Springer Physics Proceedings Vol. 58 (Springer, Berlin, 1992), pp. 183–186.
[7] F. Haake, M. Kuś, and R. Scharf, Z. Phys. B **65**, 381 (1987).
[8] J. L. Martin, Proc. R. Soc. London Ser. A **251**, 536 (1959).
[9] A. Peres, *Quantum Theory: Concepts and Methods* (Kluwer, Dordrecht, 1993), p. 300.
[10] A. Peres, in *Quantum Chaos: Proceedings of the Adriatico Research Conference on Quantum Chaos*, edited by H. A. Cerdeira, R. Ramaswamy, M. C. Gutzwiller, and G. Casati (World Scientific, Singapore, 1991), pp. 73–102.
[11] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), p. 82.
[12] B. O. Koopman, Proc. Natl. Acad. Sci. U.S.A. **17**, 315 (1931).
[13] P. R. Halmos, *Lectures on Ergodic Theory* (Chelsea, New York, 1956), pp. 34–46.
[14] V. I. Arnold and A. Avez, *Ergodic Problems of Classical Mechanics* (Benjamin, New York, 1968), p. 17.
[15] E. P. Wigner, *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* (Academic, New York, 1959), p. 167.
[16] M. Tinkham, *Group Theory and Quantum Mechanics* (McGraw-Hill, New York, 1964), p. 110.
[17] A. Peres and D. Terno, Phys. Rev. E **53**, 284 (1996).
[18] F. M. Izrailev, Phys. Lett. A **134**, 13 (1988); J. Phys. A **22**, 865 (1989).
[19] J. Ford, in *Chaotic Dynamics and Fractals*, edited by M. F. Barnsley and S. G. Demko (Academic, New York, 1986), pp. 1–52.