Apparent randomness in quantum dynamics

Hilda A. Cerdeira
Instituto de Física, Universidade Estadual de Campinas, 13081 Campinas, São Paulo, Brazil

B. A. Huberman
Xerox Palo Alto Research Center, Palo Alto, California 94304
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We show how bounded quantum systems in the presence of time-periodic fields can mimic random behavior in spite of their almost periodic character. We calculate the distribution of values taken by observables in the course of time, and demonstrate how they become asymptotically Gaussian in the large-N limit but with constant variance and *a posteriori*, δ-correlated noise. Thus, unlike *a priori* processes, the quantum dynamics of bounded systems remains nondiffusive while appearing to be random.

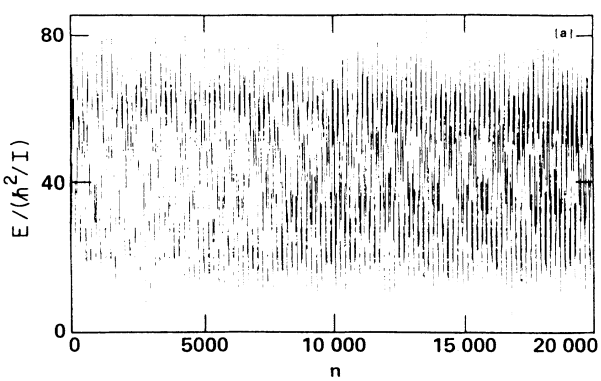
I. INTRODUCTION

The statistical behavior of observables in quantum dynamics is of relevance to many problems in physics and chemistry.[1-3] In particular, the existence of classical systems which exhibit chaotic behavior poses interesting questions about the dynamics of their quantum counterparts.

For systems with time-independent Hamiltonians, the notion of nonintegrability in quantum dynamics is usually associated with the statistical distribution of energy-level spacings, which in the case of systems with classically chaotic counterparts, exhibit level repulsion.[4-8] These results, relying mostly on numerical calculations, show that the distribution of energy levels agrees with the statistics of Gaussian orthogonal ensembles (GOE) for time-reversal–invariant systems, while displaying statistics of Gaussian unitary ensembles (GUE) in problems without time-reversal invariance.[9]

The problems associated with the dynamics of quantum systems whose Hamiltonians are time dependent are of a different nature from those discussed above. In particular, the study of their energy spectra is not sufficient to elucidate the nature of their dynamics. One of the early criteria for the existence of quantum chaos in such systems, proposed by Casati *et al.*, was borrowed from similar concepts in classical Hamiltonian dynamics.[10] Specifically, the appearance of diffusive behavior in the time evolution of observables such as the expectation value of the energy was proposed as a test of the existence of chaotic dynamics. This criterion, which was tentatively identified in early numerical simulations of the quantum-kicked rotor, was discarded when it was shown that the very nature of quantum dynamics precludes such behavior. Rather, for any periodically driven system with a point-energy spectrum, both the wave function and the observables behave in an almost periodic fashion, implying recurrent behavior which, although possibly ergodic, is not mixing.[11]

Regardless of the above limitations, an interesting question concerns the statistical properties of the time evolution of observables in experiments probing the dynamics of quantum systems in the presence of external periodic fields. In other words, one may ask the following: How does the data look? Regular or random in time? Such questions can be illustrated with the example of Fig. 1(a),



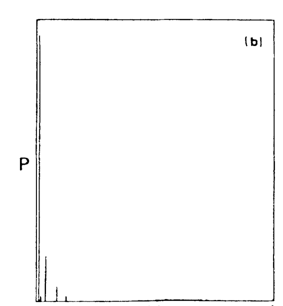


FIG. 1. (a) Expectation value of the energy E divided by $\hbar^2/I$ as a function of the number of pulses applied to the quantum rotor. The system was initially in the ground state and the parameter values were $k=2.871$ and $\tau=2.532$. A total of 201 states were used in the computation. See Ref. 11. (b) Power spectrum for the quantum system of Fig. 1(a). 8192 iterates were used and the dc component removed. T is the time between pulses.

where the time evolution of the energy for the quantum-kicked rotor is shown for the first 20.000 pulses. In spite of its random appearance, it Fourier transform, shown in Fig. 1(b), shows that it is a quasiperiodic function composed of five frequencies. As we will show, in spite of their recurrent behavior, the dynamics of observables can pass many of the tests which are used to characterize random signals. Thus, short of a Fourier analysis of the time series, quantum systems in the presence of periodic fields can mascarade as chaotic ones.

In what follows, we will consider the time evolution of a bounded quantum system, subjected to a time-periodic potential. It is well known that the behavior of the wave function, as well as that of the energy, is an almost periodic function.[11] Moreover, since the ratios between the corresponding quasienergies are dense in the irrationals, the observables return arbitrarily close to their initial values infinitely often, regardless of the initial configuration of the system. We will first consider a system whose number of energy levels N is finite and study the behavior of the time-dependent values of the energy as N approaches infinity. We will then show that the distribution becomes asymptotically Gaussian, with constant variance and *a posteriori*, δ-correlated nonwhite noise. This in turn implies that contrary to some conjectures, the process remains nondiffusive although the observable may appear to be random.

II. STATISTICAL PROPERTIES OF OBSERVABLES

A. The distribution function

Although the time dependence of the Hamiltonian is not necessary for what follows, we will consider the case when it is periodic in time and bounded, with a pure point spectrum.[12] Let

$$H(t)=h_0+V(t) , \tag{1}$$

with

$$H(t+\tau)=H(t) . \tag{2}$$

Using Floquet's theorem, it can be shown that the solution of the Schrödinger equation can be written as[13]

$$\psi(t)=\sum_k \phi_k(t)e^{i\varepsilon_k t/\hbar} , \tag{3}$$

where

$$\phi_k(t)=\phi_k(t+\tau) , \tag{4}$$

ε_k is the quasienergy, and $\phi_k(t)$ the quasiperiodic state, which obeys the equation

$$[H(t)-\varepsilon_k]\phi_k(t)=i\hbar\frac{\partial\phi_k}{\partial t} . \tag{5}$$

In this case, if the quasienergies form a discrete set and the potential is bounded, it is well known that, away from resonances, the system behaves in a recurrent, almost periodic fashion.[11] Numerical experiments also indicate that the existence of these resonances will not prevent the system from reassembling itself.

When the quasienergy spectrum is pure point and finite, although large, and the ratio between the quasienergies is irrational, the wave function is almost periodic.[11,14] In order to elucidate the behavior of the system with an infinite spectrum, we calculate the probability distribution of an observable around a mean value. Although we focus our attention on the energy, our results apply to any observable of the system. The general form of the energy for an N-level system can be written as

$$E_N(t)=\sum_{n=1}^{N} C_n \cos\theta_n ,$$
$$\theta_n=\omega_n t+\phi_n \pmod{2\pi} , \tag{6}$$

where $\omega=\varepsilon_n/\hbar$. The quantities ε_n, C_n, and ϕ_n can be calculated using the method of Cerdeira *et al.*[14] Furthermore, since the ε_n are all real, the C_n's are time independent. Notice that when the time dependence of the Hamiltonian is such that one cannot perform a canonical transformation to make it time independent, the C_n's can become, in principle, functions of time and therefore could give rise to diffusive behavior. In that case, the ε_n's and the C_n's can be calculated using a method developed by Otero *et al.*[15]

Let us define a characteristic function of the distribution of the random variable

$$f_N(x)=\langle e^{ixE_N}\rangle=\int \prod_{n=1}^{N} e^{ixC_n F(\theta_n)}\frac{d\theta n}{2\pi} , \tag{7}$$

where

$$F(\theta_n)=\cos(\omega_n t+\phi_n) , \tag{8}$$

with Lebesgue measure.[16,17] The characteristic function can be written as

$$f_N(x)=\prod_{n=1}^{N} J_0(C_n x) , \tag{9}$$

where $J_0(x)$ is a Bessel function. The probability density distribution is defined as the Fourier transform of $f_N(x)$ in the limit $N\to\infty$, i.e.,

$$P(E)=\lim_{N\to\infty} P_N(E) \tag{10}$$

and such that

$$P_N(E)=\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ixE}f_N(x)dx \tag{11}$$

or

$$P_N(E)=\frac{1}{2\pi}\prod_{n=1}^{N}\int_{-\infty}^{\infty} dx\, e^{-ixE}J_0(C_n x) . \tag{12}$$

This in turn, can be expressed as

$$P_N(E)=\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{-ixE} \times \exp\left[-\left[\sum_{n=1}^{N} -\ln J_0(C_n x)\right]\right] . \tag{13}$$

Since for large values of the argument $[\ln J_0(C_n x) < 1]$ the integral converges, we can use the method of steepest descents in the large-N limit. The condition for the existence of an extremum is given by

$$\sum_{n=1}^{N} C_n \frac{J_1(C_n x)}{J_0(C_n x)} = 0 .$$

Since the sum is not zero at any point other than $x = 0$, we can take this as the only significant minimum. To lowest order in x we find

$$P_N(E) = \frac{1}{\sqrt{2\pi}\sigma_N} \exp(-E_N^2/2\sigma_N^2) , \quad (14)$$

where

$$\sigma_N^2 = \tfrac{1}{2} \sum_{n=1}^{N} C_n^2 \quad (15)$$

and

$$P(E) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-E^2/2\sigma^2) . \quad (16)$$

From Eq. (16) it follows that σ^2 is the variance, which is time independent. However, the quantity $P(E)$ is a Gaussian distribution centered at $E = 0$. We therefore notice that since Eq. (16) is the limit of the distribution as $N \to \infty$, the recurrence of E will only be determined by the convergence of σ_N to a finite value.

B. Corrections to the Gaussian distribution

Let us now estimate the corrections to the Gaussian distribution due to finite N. Expanding the $\ln J_0(C_n x)$ around the saddle point we can write Eq. (13) as

$$P_N(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx\, e^{-ixE} \exp\left[\frac{x^2\sigma_N^2}{2} - \alpha_{N,4} x^4 - \alpha_{N,6} x^6 - \cdots \right] , \quad (17)$$

where

$$\alpha_{N,4} = \tfrac{3}{8} \sum_{n=1}^{N} \frac{C_n^4}{4!} , \quad (18a)$$

$$\alpha_{N,6} = \tfrac{5}{4} \sum_{n=1}^{N} \frac{C_n^6}{6!} , \quad (18b)$$

and in general

$$\alpha_{N,m} = \text{const.} \times \sum_{n=1}^{N} C_n^m .$$

Expanding Eq. (17) to order x^6 and completing the square,

$$P_N(E) = \frac{e^{-E_N^2/2\sigma_N^2}}{2\pi} \int_{-\infty}^{\infty} dy\, e^{-\sigma_N^2 y^2/2} [1 - \alpha_{N,4}(y - iE_N/\sigma_N^2)^4 - \alpha_{N,6}(y - iE_N/\sigma_N^2)^6 - \cdots] . \quad (19)$$

After some manipulation, $P_N(E)$ reduces to

$$P_N(E) = \frac{e^{-E_N^2/2\sigma_N^2}}{2\pi\sigma_N} \left[1 - \frac{\alpha_{N,4}}{\sqrt{\pi}} \left[\frac{\sqrt{2}}{\sigma_N}\right]^4 \int_{-\infty}^{\infty} dt \left[it + \frac{E_N}{\sqrt{2}\sigma_N}\right]^4 e^{-t^2} + \frac{\alpha_{N,6}}{\sqrt{\pi}} \left[\frac{\sqrt{2}}{\sigma_N}\right]^6 \int_{-\infty}^{\infty} dt \left[it + \frac{E_N}{\sqrt{2}\sigma_N}\right]^6 e^{-t^2} - \cdots \right] . \quad (20)$$

This equation can be written in terms of the Hermite polynomial

$$P_N(E) = \frac{e^{-E_N^2/2\sigma_N^2}}{\sqrt{2\pi}\sigma_N} \left[1 - \frac{\alpha_{N,4}}{(\sqrt{2}\sigma_N)^4} H_4\left[\frac{E_N}{\sqrt{2}\sigma_N}\right] + \frac{\alpha_{N,6}}{(\sqrt{2}\sigma_N)^6} H_6\left[\frac{E_N}{\sqrt{2}\sigma_N}\right] - \cdots \right] . \quad (21)$$

In order to study the convergence of $P_N(E)$ as $N \to \infty$, we need to determine the behavior of expressions like

$$\frac{\sum_{k=1}^{N} C_k^{2n}}{\left[\sum_{k=1}^{N} C_k^2\right]^n} , \quad n \geq 2 \quad (22)$$

which, except for the constant factor in front of $\alpha_{N,2n}$, are the coefficients of $H_{2n}(x)$ and depend only on n. Considering first the simplest case, $C_k = C$, for all k's, Eq. (22) then becomes

$$\frac{NC^{2n}}{(NC^2)^n} = \frac{1}{N^{n-1}} . \quad (23)$$

Since the argument of the Hermite polynomials also vanishes with a constant variance, Eq. (21) converges to a

Gaussian for $N \rightarrow \infty$. It is therefore clear that in the case when all C_k's are different, all terms in Eq. (21) will converge faster than the criteria given by Eq. (23).

The next task consists in finding the second-order correlation function, or covariance, of the random variable $E_N(t)$, as $N \rightarrow \infty$. It is defined as

$$C_N(\sigma) = \langle E_N E_n \rangle - (\langle E_N \rangle)^2 = \langle E_N E_N \rangle .$$

Since the statistical characteristics of the process are invariant under time shifts, the process is stationary, which implies that $C_N(\tau)$ is determined by[17]

$$C_N(\tau) = \lim_{T \rightarrow \infty} \left[\frac{1}{T} \int_0^T E_N(t) E_N(t+\tau) dt \right] . \quad (24)$$

This integral can be easily calculated to give

$$C_N(\tau) = \sum_{n=1}^{N} \frac{C_n^2}{2} \cos(\omega_n \tau) , \quad (25)$$

which is again an almost periodic function of τ. If we now calculate the dimensionless, normalized correlation coefficient $R(\tau)$ defined as[17]

$$R(\tau) = \frac{\langle C_N^2(\tau) \rangle}{\langle C_N^2(0) \rangle} = \begin{cases} 1, & \tau = 0 \\ \dfrac{\sum_{n=1}^{N} \frac{C_n^4}{8}}{\left[\sum_{n=1}^{N} \frac{C_n^2}{2} \right]^2} \rightarrow \dfrac{1}{N} \quad \text{as } N \rightarrow \infty & \\ \tau \neq 0, & \end{cases} \quad (26)$$

we can use it to determine the conditional variance of an *a posteriori* random process and which is given by $\sigma^2[1-R^2(\tau)]$, where σ is the constant variance as defined above. The *a posteriori* processes are nonstationary, δ correlated, becoming equal to "*a priori*" ones in the limit $\tau \rightarrow \infty$.

III. CONCLUSION

In this paper we have studied the time evolution of observables for bounded quantum systems subjected to time-periodic fields. We have shown that in spite of their recurrent, almost periodic behavior, the distribution of values produced by the evolution of the observables becomes Gaussian in the large-N limit. This implies that any statistical probes short of a Fourier transform would indicate that the system appears to behave in random fashion. Notice, however, that since the variance does not grow in time, neither will the energy, thus preventing the dynamics to become chaotic in the sense of classical mechanics. This observation applies to a number of quantum dynamics problems, including the quantum-kicked rotor.[10,11,18,19]

Besides their obvious application to bounded systems subjected to time-periodic fields, these results are also relevant to the statistical distribution of energy-level spacings in time-independent Hamiltonian systems; a problem which is closely related to the integrability of their classical counterparts.[4–9] This can be seen by noticing that the spectral distribution of GOE or GUE systems can only represent a pure point spectrum, for otherwise it would imply the existence of degeneracies. Furthermore, since the theory of random matrices applicable to these problems[9] describes *a posteriori*, δ-correlated nonwhite-noise processes, it implies that in systems with discrete, nondegenerate spectra, one will also observe a nondiffusive Gaussian distribution of the random variables.

Last but not least, these results apply to a number of other problems characterized by almost periodicity. These include both classical dynamics and some other quantum systems which have been the focus of recent activity. Among the more prominent ones, we mention the problem of electron behavior in quasiperiodic potentials produced by either the static atomic configuration of a quasicrystal, or by the frozen configuration of phonons which a swift electron would sample in a perfect solid. In all these cases, the quasiperiodic behavior of the potential can always mimic a random process which is nevertheless nondiffusive.

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