# Dynamical Stability of Quantum "Chaotic" Motion in a Hydrogen Atom

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A simple numerical reversibility test which proves useful in exposing the chaotic nature of classical dynamical systems is applied to the quantum model of a hydrogen atom in a microwave field. The remarkable result is that, in spite of some apparent chaotic features, the quantum motion proves to be perfectly stable in contrast to the high instability of the classical chaotic motion.

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The crucial way in which exponential instability of orbits affects macroscopic reversibility is theoretically well understood. In particular, it implies that nonequilibrium statistical ensembles evolve in time towards equilibrium. This approach to equilibrium does in no way contradict the strict reversibility of the equations which describe evolution of phase densities. Indeed, by integration backwards of the Liouville equation, the initial distribution would eventually be reassembled; nevertheless, should this integration be continued still further in the past, an equilibrium distribution would again be approached.

It is an impressive demonstration of the unwieldy character of exponential instability that this reversal of time evolution cannot be carried out in practice on computer experiments, where, through inevitable numerical errors, the memory of the initial distribution is completely lost after a while. Thus the numerically computed time evolution will not reproduce backwards the history of the system, except for a short time; afterwards, approach to equilibrium will again show up, and the initial distribution will be lost forever. Needless to say, the exactly computed evolution would in any case find its way back to the original state; therefore, in order to explain irreversible macroscopic behavior one must resort to some kind of coarse graining.

However, this lack of "practical" reversibility is a distinctive mark of true dynamical chaos.[1,2] Its appearance in computer experiments unambiguously hints at a quite complex and sensitive nature of orbits.

The question of whether or not chaos persists in quantum dynamics has already been the object of many investigations.[3] At the present state of knowledge, quantum mechanics places severe limitations on the classical chaotic properties of the motion. In this paper, we will inquire about the existence of any "practical" irreversibility of quantum motion; as a result, we will be able to give one more illustration of quantum suppression of dynamical chaos.

Numerical experiments on time reversal of quantum evolution of classically chaotic systems were already described by Shepelyansky[4] for the so-called "kicked rotator" model. Evidence was given there that whereas the classical rotator is chaotic and practically irreversible the quantum rotator is not, and its evolution can be traced back to the initial state just by reversal of phases in the Fourier expansion of the wave packet (velocity reversal). Even more remarkably, this reversibility is substantially unaffected by any small change in the phases before reversal. Here we present results of similar numerical experiments on another quantum system subjected to a time periodic perturbation: the one-dimensional model of a hydrogen atom in a monochromatic field. Our motivation is not only to give another, more physical, example of quantum stability. A more important point is that the kicked rotator is a very special model in that the quantum motion is known to be always localized (in momentum space) which implies a pure point quasienergy spectrum and a recurrent quantum evolution. Strictly speaking, there are values of the external period, both resonant and nonresonant, which give rise to a continuous spectrum.[5] However, the localization picture looks fairly general.

Thus one may have some doubts as to whether quantum stability would persist even in those quantum systems where the localization phenomenon is absent. This is just the case for the one-dimensional hydrogen atom, where we are faced with a more complex and general situation. In particular, the quasienergy spectrum is here known to be continuous, which is especially obvious in case of delocalization. As is well known, continuity of the spectrum is a necessary feature of classical chaotic motion.

Let us consider the one-dimensional model of the hydrogen atom in an external monochromatic, linearly polarized, electric field specified by the Hamiltonian

$$H = p^2/2 - 1/x + \epsilon x \cos(\omega t), \quad x > 0, \tag{1}$$

where $\epsilon$ and $\omega$ are the field strength and frequency in atomic units.

It is known that the classical system undergoes a transition from regular to chaotic motions[6,7] as the strength of the external field exceeds a critical value $\epsilon_c = \epsilon n_0^4 \approx 1/50\omega_0^{1/3}$ (where $\omega_0 = \omega n_0^3$ is assumed to be $\geqslant 1$ and $n_0$ is the initial action corresponding to the principal quantum number of the hydrogen atom). In this region the motion can be approximately described by a diffusion in action space obeying the Fokker-

 

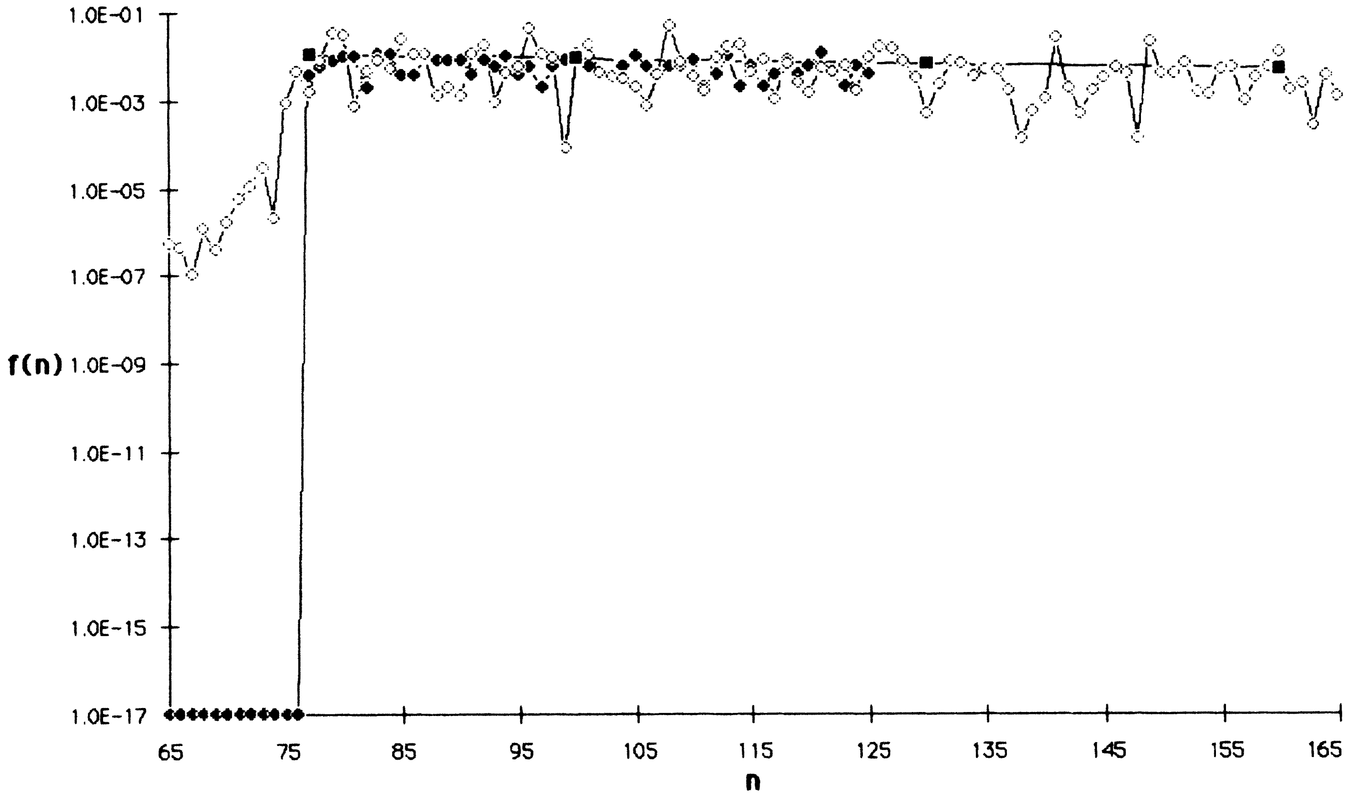


FIG. 1. Probability distribution on unperturbed states after $\tau=60$ periods of the microwave field for the classical (solid lozenges) and the quantum (open lozenges) system. Here, $n_0=100$, $\omega_0=1.5$, $\epsilon_0=0.08$. Notice the fairly good agreement between classical and quantum numerical results and the analytical solution given by Eq. (3) (squares).

Planck equation:

$$\frac{\partial f(n,\tau)}{\partial \tau}=\frac{\partial}{\partial n}\left[D(n)\frac{\partial f(n,\tau)}{\partial n}\right], \tag{2}$$

where

$$D\approx 2\epsilon_0^2 n^3/\omega_0^{7/3}n_0=2\epsilon^2 n^3/\omega^{7/3}$$

and $\tau=\omega t/2\pi$ is the dimensionless time measured in the number of field periods.

In the quantum case another critical field strength was shown to exist, the *quantum delocalization border*[8]: $\epsilon_q\approx\omega_0^{7/6}/(6n_0)^{1/2}$. Below this value quantum effects lead to a limitation of classical diffusion within a finite interval of $n$ values. For field strengths above the quantum border $\epsilon_q$ the diffusive excitation becomes unbounded and is again approximately described by the classical diffusion equation (2).

We performed the reversibility test with parameters and initial conditions above the delocalization border: $n_0=100$, $\epsilon_0=0.08$, $\omega_0=1.5$. In this way we provide the maximal chaos possible in a quantum system. Similarly to the quantum case where the single unperturbed state $n_0=100$ was excited, in the classical computations we chose the same parameters and analogous initial conditions. Namely, we computed 1000 trajectories with the same initial action $n_0=100$ and phases uniformly distributed within the interval $[0,2\pi]$.

In order to simulate the quantum evolution numerically we made use of a Sturm basis which allowed us to take into account transitions to, from, and within the continuous spectrum. The details and checks of our numerical technique will be described elsewhere.[9] The numerical computations have been done on a Cray XMP computer. Our Sturm basis consists of 448 vectors that, notwithstanding their square-integrable nature, include a significant part of the continuous spectral subspace of the unperturbed atom. An important remark is that no expansion approach can be applied in order to integrate the Liouville equation because the relevant basis set would increase exponentially in time.

In Fig. 1 we show the probability distribution on unperturbed states after $\tau=60$ periods of the microwave field for both classical and quantum systems as well as the approximate analytical solution of the classical diffusion equation (2):

$$f(y,\xi)\approx\frac{1}{2y^{3/4}(\pi\xi)^{1/2}}\left\{\exp\left[-\frac{(1/\sqrt{y}-2/\sqrt{y}+1)^2}{\xi}\right]+\exp\left[-\frac{(1/\sqrt{y}-1)^2}{\xi}\right]\right\}, \tag{3}$$

where $y = n/n_0$, $\bar{y} = \bar{n}/n_0$, $\xi = 2\tau\epsilon_0^2/\omega_0^{7/3}$. The solution (3) holds for $\xi/\sqrt{y} << 1$ only and corresponds to the boundary condition $(\partial f/\partial n)_{n=\bar{n}} = 0$ at the value $\bar{n}$ given by classical numerical simulations.

The sharp drop of the probability distribution at $n = \bar{n} = 76$ is due to the stability of classical motion for $n < \bar{n}$.[6] From Fig. 1 it is seen that, on the average, the quantum behavior follows the classical one which, in turn, is in satisfactory agreement with the solution of the diffusion equation. In this situation the classical motion is known to be highly unstable. Will the same be true for a similar looking quantum motion? To answer this question we applied the reversibility test discussed above. Namely, at time $\tau = 60$ we reversed the velocities in both the classical and quantum systems and followed the evolution for another sixty field periods. The result is shown in Fig. 2. Now, unlike Fig. 1, we see a striking difference between the classical and quantum behavior. In the former case there is no sign of reversibility, as expected, because of the strong instability of classical motion. Moreover, the new distribution in Fig. 2 again agrees with the theoretical curve for $\tau = 120$ (see also in Fig. 3). In contrast, the quantum motion proves to be almost completely reversible and this implies, however strange it may seem, that the quantum dynamics is stable even though it is diffusive. An interesting conclusion can be drawn from this: Unlike classical chaotic motion, the past history of a quantum system can always be recovered from its present state.

A different illustration of this reversibility phenomenon is given in Fig. 3 where the excitation probability is shown as a function of time $\tau$. The specular symmetry of the quantum curve about the time of reversal $\tau = 60$ again demonstrates the reversibility and stability of the diffusive quantum motion. In contrast, the strong instability of the classical motion leads to a continuation of the diffusion process after velocity reversal (obviously except for a short time interval).

We emphasize that the reversibility phenomenon does not depend on the particular initial condition which we used in this paper simply as an example.

The reversibility of the quantum motion is even more spectacular if we notice that part of the recovered initial state comes back from the continuum (see Fig. 3). The latter process is a peculiar kind of a coherent recombination.

Thus quantum mechanics provides an interesting example of a dynamically stable diffusion. Of course, this process is by no means a truly chaotic (random) process[1,2]; nevertheless, it is characterized by strong, important, statistical properties. In this connection the interesting question arises whether stronger statistical properties are necessary at all for statistical mechanics.[10]

We notice that a similar situation may happen also for some classical system, for example, for linear waves in cavities so shaped as to behave like chaotic billiards in the geometrical-optics limit.

This interesting phenomenon of stable diffusion suggests a reconsideration of some fundamental problems in the nature of classical and quantum mechanics.

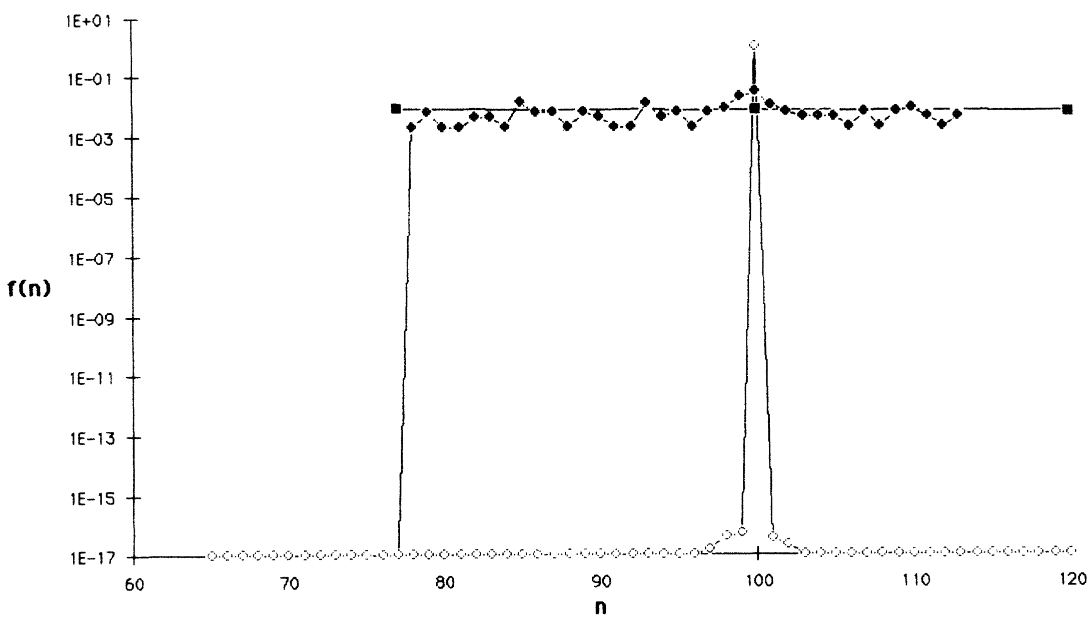


FIG. 2. Probability distribution on unperturbed states at $\tau = 120$ for the case of Fig. 1, after reversal of velocities at $\tau = 60$. Notice that the quantum system (open lozenges) recovers its initial state to seventeen digits which corresponds to numerical errors. In contrast, the classical motion (solid lozenges) proceeds according to the diffusion equation (2) (squares).

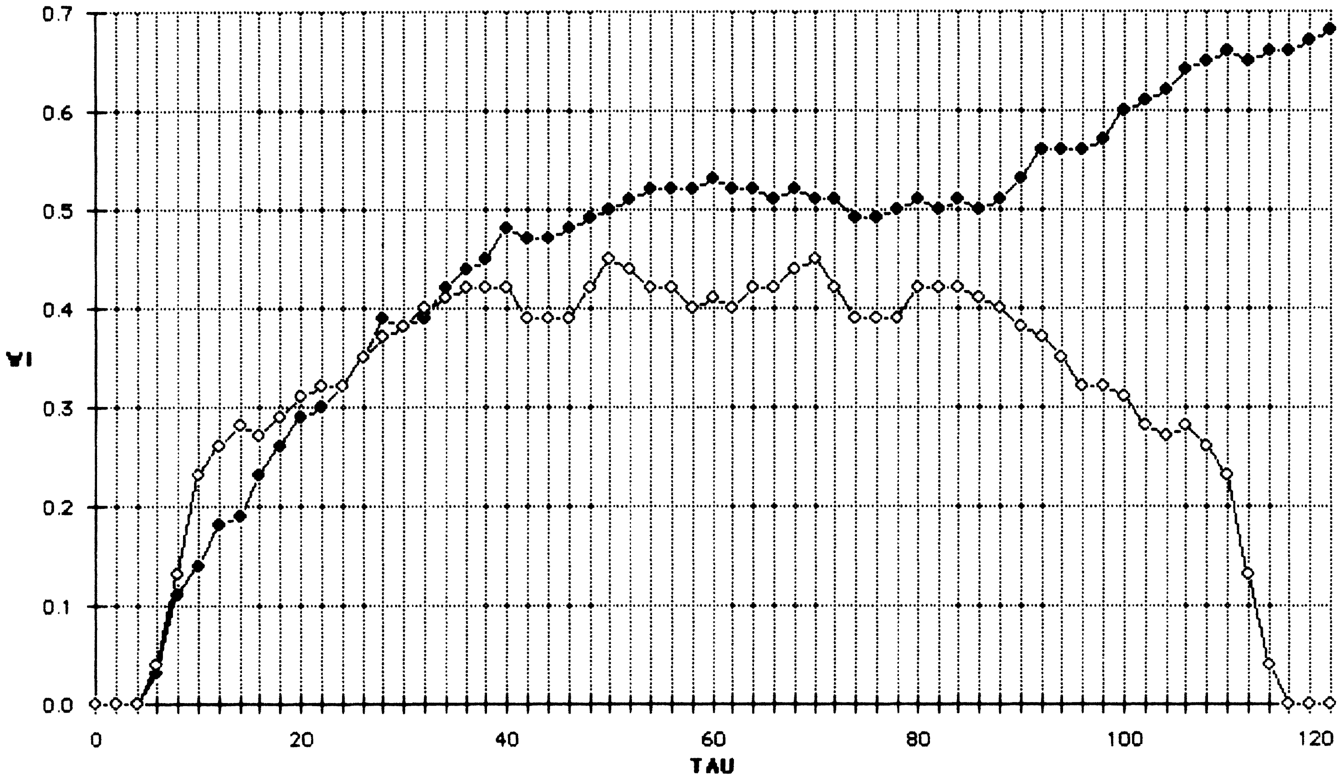


FIG. 3. Classical (solid lozenges) and quantum (open lozenges) ionization probability (excitation above the unperturbed level $n = 150$) as a function of time $\tau$ for the case of Fig. 2. Notice the perfect specular symmetry of the quantum curve about the time of reversal $\tau = 60$.

Until recently, classical motion was considered to be, in principle, perfectly predictable; however, we are now aware that, because of dynamical chaos, classical mechanics also possesses some inherently statistical features. On the other hand, quantum mechanics is still understood as an intrinsically statistical theory. Yet, on account of the stable character of "quantum chaos," quantum dynamics must now be acknowledged a much more deterministic character than classical dynamics. Of course, the quantum measurement process remains irreversible and inevitably statistical, so that we see here an additional reason to distinguish the measurement process from the proper quantum dynamics. As a matter of fact, the latter is much more stable and less chaotic than classical dynamics.

However, it would be misleading to think that the stability of quantum dynamics is only due to the exclusion of measurements. Indeed, this stability clearly manifests itself, for example, in the localization phenomenon which can be easily observed in laboratory experiments.[8]

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