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Theory of Chaos in the Atomic Hydrogen

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1. Introduction

Investigations on the possibility of quantum chaotic behaviour have now grown into an autonomous field of research, usually referred to as 'Quantum Chaos' /1,2/. Arguments under current investigation range from issues of a mostly foundational flavour to others directly related to the phenomenology of microsystems. Indeed, some very actual problems in Quantum Chaos are of direct interest to molecular and atomic physics, to solid state physics and to quantum optics. Such problems are currently being investigated in close connection with experimental research and are of major applicative interest.

One central problem of Quantum Chaos is the applicability of classical nonlinear models to microphysical systems in the atomic and molecular domains. This is an important point, because classical models often exhibit quite peculiar dynamical properties, connected with the onset of chaos. For example, classical models for atoms in microwave field or molecules in laser fields predict that, for sufficiently high fields, a regime of chaotic motion is entered, characterized by a diffusion in phase space eventually leading to ionization. This diffusive phenomenology would be quite beyond the qualitative predictions of standard quantum mechanical treatment.

As is known, chaotic motion in classical mechanics is a fairly general occurrence when an integrable system is subject to some perturbation. The latter can be both time-independent and time-dependent; in the latter case, it is important to remark that the appearence of chaos does not require any particular disorder in the time dependence of the perturbation; even a periodic perturbation may be effective in this sense.

The onset of chaos has usually a threshold-like character in the perturbation strength and modern ergodic theory provides a clean

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mathematical framework for the mechanism of chaos generation; nevertheless, effective estimates of chaotic thresholds and quantitative descriptions of chaotic motion rely on at least partially heuristic criteria and/or on computer simulations.

The dynamical chaos is of absolute relevance, both for theory and applications. In the first place, the fact that chaotic motion is in many respects practically indistinguishable from a pure stochastic motion , raises important questions about the deterministic nature of classical mechanics. On the other hand, chaos involves a very peculiar phenomenology; e.g., in case that the perturbation is time-dependent, it may lead to indefinite diffusion in phase space with obviously observable consequences. Classical models for microphysical systems are usually of this type, i.e., they exhibit a stochastic transition. It is then a fundamental problem to understand what happens upon quantizing such models.

Two classes of problems should be distinguished:

1) Conservative systems described by time-independent Hamiltonians.
2) Systems under time-periodic or quasi-periodic perturbations.

The question of persistence of classical chaos in the first class of problem has been rather extensively studied and the general answer is known to be negative, simply because conservative bounded quantum systems have in all cases a pure point energy spectrum; this implies recurrent behaviour of any observable, in sharp contrast with the nonrecurrent classical dynamics, which is associated with a continuous spectrum. There is of course no violation of the correspondence principle involved here because, in the semiclassical regime, the quantum dynamics does indeed reproduce the classical behaviour, over some finite time scale.

However it is important to stress that the complexity of classical motion appears here in the statistical distribution of eigenvalues and eigenfunctions.

For the second class of problems, the present state of knowledge can be summarized as follows:

a) Quantum mechanics has in general an inibitory effect on classical chaos. This inibitory mechanism is closely connected to the localization phenomenon that plays a central role in solid state physics and which is

typical for wave propagation in random media: wave packets propagating in an infinite (statistically) homogeneous random medium do neither travel to infinity as they would in free space, nor do they spread indefinitely. Instead, they remain localized in essentially finite regions of space. No dissipative mechanism is involved in this phenomenon, which is in fact produced by complicated interference of partial waves randomly scattered at various places.

b) The quantum inhibition of classical chaos may not be a complete one: a more or less marked memory of the classical chaotic motion may survive in the quantum domain. Indeed, the existence of a kind of quantum regime retaining some features of classical chaotic diffusion is the only possible explanation for some experimental results by Bayfield and Koch on microwave ionization of highly excited atoms /3/.

In the following we present a theoretical analysis which leads to the understanding of the mechanism of excitation and ionization of hydrogen atoms under microwave fields. One of the main predictions of this analysis, namely the localization phenomenon, has been recently observed in laboratory experiments /4,5/.

2. The Kicked Rotator

In order to understand the modifications that quantum mechanics imposes on the classical picture of chaotic motion it is convenient to start from a model which is sufficiently simple but which display the typical, very rich behaviour of classical systems: the δ-kicked rotator. This model is described by the Hamiltonian:

$$H = p^2/2 + \omega^2 \cos\theta \sum_n \delta(t-nT) \qquad (1)$$

where p is the rotator momentum, θ is the angular coordinate, T the kick period and ω the perturbation strength.

In classical mechanics, the study of this model has provided deep insight into the general behaviour of dynamical systems, since it shares almost all their main features. Correspondingly, one may expect that the study of the quantum properties of the kicked rotator, especially in regions of

parameters where the corresponding classical model is chaotic, will be of great relevance for understanding the qualitative features of the quantum motion.

Due to the presence of the δ-function, the classical equations of motions for system (1) can be integrated and reduced to the mapping:

$$P_{n+1} = P_n + K\sin\theta_n$$
$$\theta_{n+1} = \theta_n + P_{n+1} \qquad (2)$$

where $K = \omega^2 T$, n is time measured in number of kicks and P is the dimensionless angular momentum $P_n = p_n T$.

Mapping (2) is the well-known "standard map", extensively discussed in the literature and frequently used, at a tutorial level, to illustrate the great complexity of motion of simple dynamical systems. Indeed the motion of system (1) presents completely different qualitative features depending on whether K is less or larger than $K_c \sim 1$. More precisely for $K<K_c$ most orbits lie on smooth curves and , in particular, the kinetic energy remains bounded with a variation $\Delta P \sim K$. Instead, when K exceeds the critical value K_c, the mapping orbits become chaotic and the system mimics a random walk in momentum space leading to a diffusive growth of the kinetic energy:

$$\bar{P}^2 \sim (K^2/2)\, n \qquad (3)$$

and to the angular momentum distribution of the Gaussian type

$$f(P,n) = (K^2 \pi n)^{-1/2} \exp(-P^2/K^2 n) \qquad (4)$$

In order to turn to the quantum description, we write the quantum Hamiltonian:

$$H = \hbar^2 \partial^2/\partial\theta^2 + \omega^2 \cos\theta \sum_n \delta(t - n T) \qquad (5)$$

Then letting

$$\psi(\theta,t) = \sum_s c_s e^{is\theta} \qquad (6)$$

we may write the solution of the Schroedinger equation as a mapping for the wave function over one period.

$$\psi_{n+1}(\theta) = S\,\psi_n(\theta) = \exp(i\,k\cos\theta)\sum_s c_s \exp[i(s\theta - 2\pi s^2\tau)] \qquad (7)$$

where $k = \omega^2/\hbar$, $\tau = \hbar T/4\pi$ and n is again time measured in number of kick periods.

The quantum mapping (7) can be numerically iterated and , starting from a given set of $\{c_s(o)\}$, one may compute the probability distribution $f(s)=|c_s|^2$, the quantum average kinetic energy $\sum s^2|c_s|^2$ and compare the time dependence of these two quantities with the classical one given by eqs. (4) and (3) respectively.

Surprisingly enough, it turned out /6,7/ that in typical situations the quantum excitation would follow the classical pattern only up to a finite time t_B, called break-time, after which the quantum rotator appears to enter a stationary regime, where the average kinetic energy oscillates around a maximum value. In this stationary regime, the quantum distribution over eigenstates of the free rotator is "frozen", the excitation decreasing exponentially away from the initially excited state /7,8/.
This "saturation" in the energy growth was qualitatively and quantitatively explained by the pure-point nature of the quasi-energy (q.e.) spectrum /9,10/ which is essentially the spectrum of operator S in (7). Indeed, in the quantum system, diffusive excitation can take place on a time scale so small that the wave packet evolution cannot "perceive" the finite separation of quasi-energy eigenvalues. Therefore, if ΔE is the average spacing of the q.e. eigenvalues represented in the wave packet, the break-time should be defined in order of magnitude by $t_B\,\Delta E \sim \hbar$.

Moreover, a formal connection between the rotator problem and the one-dimensional tight-binding model with a time-independent pseudorandom potential was found /8/, which led to the recognition that the quantum suppression of the chaotic excitation of the rotator is a sort of a dynamical version of Anderson localization. Therefore, the most important lesson learned from the kicked-rotator model was that the classical diffusive excitation, taking place above the chaotic threshold, is quantum mechanically suppressed by interference effects that lead to exponential localization of excitation in momentum space.

3. The Hydrogen Atom

The main question now is whether this phenomenon of quantum suppression of classically chaotic diffusion is peculiar of the kicked rotator model or a general occurrence in quantum mechanics.
A seemingly negative indication was given by the analysis of a completely different problem, namely, the microwave ionization of highly excited hydrogen atom. Indeed, in laboratory experiments /3/ a strong ionization was observed by making a beam of hydrogen atoms prepared in states with initial quantum number n_0=66 traverse a microwave cavity of frequency $\omega/2\pi \approx$ 10GHz and peak intensity $\epsilon \approx$ 10V/cm. In this situation, ionization would required the absorption of about 100 photons. Theoretical analysis and numerical simulations showed that a classical model satisfactorily accounts for the experimental results.

Moreover, recent laboratory experiments /11/ showed a good agreement with classical numerical computations at least for microwave frequencies such that $\omega_0=\omega n_0^3<1$, with the initially excited state n_0 in the range 40-90. Experiments with $\omega_0>1$ were not available until recently; however, it was considered quite unlikely that the localization phenomenon would appear by further increasing n_0.

The Hamiltonian of the system we are discussing can be written as

$$H= p^2/2 - 1/r + \epsilon\, z \cos \omega t \qquad (8)$$

where atomic units are used: ϵ and ω are the field intensity and frequency, and the z coordinate is measured along the direction of the microwave field.

As it was recently shown /12,13/, the one-dimensional version of (8) describes with a very good approximation the main qualitative features of the excitation process of the real atom. For this simple 1-dimensional model, it was also shown /12,13/ that the classical motion, for $\omega_0=\omega n_0^3>>1$ can be approximately described by the area-preserving map

$$\bar{N} = N + k \sin\phi$$
$$\bar{\phi} = \phi + 2\pi\omega\, (-2\omega\bar{N})^{-3/2}\ ;\ k = 0.0822\pi\, \epsilon\omega^{-5/3} \qquad (9)$$

which gives the change of $N=E/\omega$ (E the energy : $E = -1/2n^2$) and $\phi = \omega t$ between two consecutive transits of the electron at the aphelion.

The interesting fact is that upon linearizing the map (9) around the initial value $N_0 = -1/(2n_0^2\omega)$ one obtains again the well known standard map:

$$\bar{N} = N + k \sin\phi$$
$$\bar{\phi} = \phi + T\bar{N} \qquad (10)$$

with $T = 6\pi n_0^5\omega^2$. It is then well known that a transition to chaotic motion occurs for (10) when $K = kT > 1$. From this, defining rescaled quantities $\epsilon_0 = \epsilon n_0^4$, $\omega_0 = \omega n_0^3$ we get the threshold for the transition to chaotic motion in the hydrogen atom model (8)

$$\epsilon_{cr} \approx 1/(49\omega_0^{1/3}) \qquad (11)$$

Therefore, if $\epsilon_0 > \epsilon_{cr}$, strong excitation and ionization takes place in the classical model (8). Moreover, by exploiting the similarity between eq. (9) and the rotator model, it has been argued, and numerically demonstrated /12,13/, that the quantum motion of the same model is localized, i.e. that the quantum excitation process leads to a steady-state distribution given in average by

$$\bar{T}(N) \approx (1/2l)(1 + 2|N-N_0|/l)\exp(-2|N-N_0|/l) \qquad (12)$$

with a localization length

$$l \approx D \approx k^2/2 = 3.33\,\epsilon^2\omega^{-10/3} \qquad (13)$$

Notice that localization described by (12) is exponential in $N = E/\omega$, i.e., in the number of absorbed photons. This localization picture is valid, provided that $l << N_I = 1/(2n_0^2\omega)$, the number of photons required for ionization. Instead, if l given by (13) becomes comparable with N_I, localization breaks down and strong ionization takes place. From the condition $l \approx N_I$ we get a threshold

$$\epsilon_q = \omega_0^{7/6}/(6.6\,n_0)^{1/2} \qquad (14)$$

In order that strong ionization may occur in the quantum model, the condition $\epsilon_0 > \epsilon_q$ must be satisfied, in addition to the classical condition $\epsilon_0 > \epsilon_{cr}$.

As hinted above, formula (11) actually holds for $\omega_0 > 1$. (This is discussed in Ref. /14/). When $\omega_0 < 1$, Eq. (11) must be suitably corrected, and for $\omega_0 \to 0$, ϵ_{cr} must approach the static field value $\epsilon_0 \sim 0.13$. The classical border is displayed in fig. 1 (dashed curve).

To summarize, our theoretical analysis of the model (8) shows that the quantum interference effects, that in the rotator case caused a complete arrest of the classical chaotic diffusion, are still at work in the hydrogen atom model. Unlike the rotator case, however, these localizing effects of a quantum origin can be overcome and strong excitation can occur more or less along the classical lines by increasing the field ϵ_0 above the delocalization border (14).

In Fig. 1 we present a numerical check of this theory. The straight line gives the critical field value for 1% ionization, computed according to the above sketched theory. We define the ionization probability as the total probability above the level $\bar{n} = 1.5 n_0$; therefore, the threshold for 1% ionization is obtained from the condition

$$0.01 = \int_{\bar{N}}^{\infty} \bar{\Gamma}(N)\, dN \qquad (15)$$

with $\bar{N} = [1/n_0^2 - 1/(1.5n_0)^2]/(2\omega)$. The rhs of eq. (15) can be computed as a function of ϵ_0 by using eq.(12); upon solving the resulting equation for ϵ_0 we get

$$\epsilon_1 \approx (0.16\, \omega^{1/6})\, \omega_0 = 0.023\, \omega_0 \qquad (16)$$

which gives the straight line in Fig. 1.

The numerically computed 1% thresholds are represented in Fig. 1 by full circles (quantum results) and empty circles (classical results). For each value of $\omega_0 = \omega n_0^3$ they were found by numerically integrating the equations of motion (quantum and classical) by increasing ϵ_0 until a 1% total

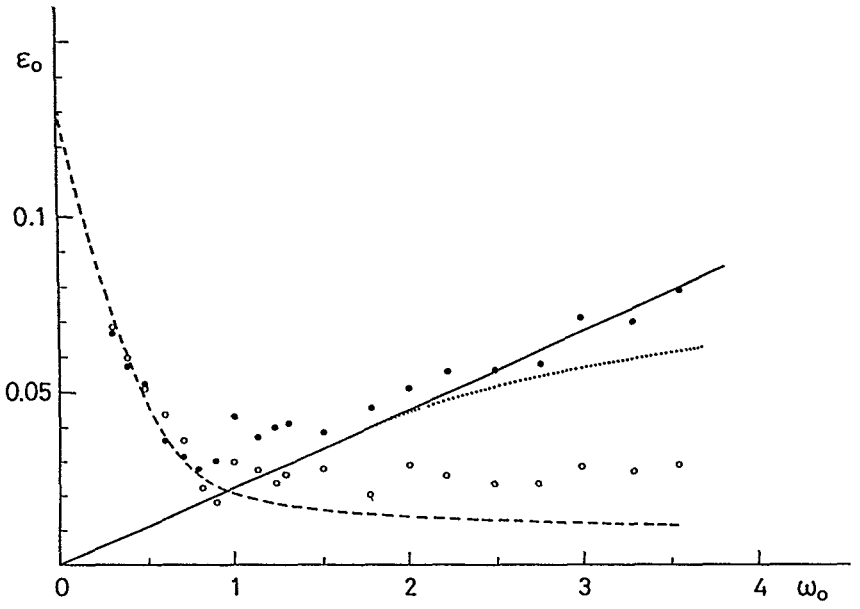

Fig. 1 - Classical (empty circles) and quantum (full circles) numerical threshold field values as a function of the rescaled frequency $\omega_0 = \omega n_0^3$, at fixed $\omega/2\pi$=26.41 GHz. The dotted curve gives the classical chaos border. The full straight line is the critical field value for 1% probability above level $\bar{n} = 1.5\ n_0$ (formula (16)). The dotted line gives the critical field for 1% probability above level n=120.

probability was reached on levels higher than 1.5 n_0. In the classical case, this probability was computed by integrating 350 orbits with given ε_0, ω_0, n_0 and homogeneously distributed phases in $(0,2\pi)$. As it is seen, for $\omega_0 > 1$, there is a quite good agreement between the quantum numerical results and our theoretical estimate (16).

It is also apparent from Fig. 1 that for $\omega_0 < 1$ the quantum excitation process closely follows the classical one /15/. This is due to the fact that for $\omega_0 < 1$ the quantum delocalization border falls below the classical chaotic threshold, so that there are no limitations of a quantum origin to the onset of chaotic excitation. The increase in the quantum numerical thresholds near $\omega_0 \approx 1$ is produced by the main resonance centered at ω_0=1; see also Fig. 5 of Ref. /14/.

Of course, our theoretical analysis is a rather crude one, and should only be expected to account for the gross qualitative features of the quantum motion. In addition to quantum localization, other effects are here at work,

such as tunneling through KAM curves, resonance effects, etc., which are responsible for the fine structure of Fig. 1.

Fig. 1 also shows that the numerically computed classical thresholds are higher than the theoretical classical border. The reason is that, whereas the theoretical curve yields the threshold for the chaotic transition, the numerical data give the critical fields for 1% ionization after τ_{ex}~400 microwave periods. According to a theoretical estimate (formula (6) of Ref. /14/) the classical ionization time is $\tau_1 \sim \omega_0^{7/3}/2\epsilon_0^2$ which, on the chaotic border $\epsilon_0 \sim 1/(49\omega_0^{1/3})$, and for $\omega_0 > 1$, takes the value $\tau_1 \sim (10\omega_0)^3 > \tau_{ex}$. Therefore, due to the small interaction time, a stronger field than ϵ_{cr} is required in order to get 1% ionization.

We would like to add one final remark concerning the comparison with experimental data. In actual laboratory experiments it may be convenient to define the ionization as the total probability above some fixed level $\overline{n}$, (and not, as in our simulation, above $\overline{n} = 1.5n_0$ dependent on the initial level n_0). The corresponding 1% thresholds should not be very different provided that n_0 is kept sufficently smaller than $\overline{n}$. For sake of comparison, in Fig.1, we also plotted the theoretical curve for 1% probability above n=120.

4. Conclusions

The main qualitative feature of our theoretical and numerical data is the suppression of chaotic excitation produced by quantum mechanics in the region $\omega_0 > 1$, where the quantum thresholds rise significantly above the classical ones. Very recent laboratory experiments /4,5/ have shown the localization phenomenon for $\omega_0 > 1$ and the experimental data are in good agreement with the original theoretical predictions /16/. This is therefore the first experimental observation of the suppression of classically chaotic diffusion produced by quantum mechanics, a fact which may turn out to be of great relevance.

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