ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

G. Casati, B.V. Chirikov,
I. Guarneri, D.L. Shepelyansky

TWO-DIMENSIONAL LOCALIZATION OF DIFFUSIVE EXCITATION IN THE HYDROGEN ATOM IN A MONOCHROMATIC FIELD

PREPRINT 87-30

НОВОСИБИРСК

Two-Dimensional Localization of Diffusive Excitation in the Hydrogen Atom in a Monochromatic Field

*G. Casati**, *B.V. Chirikov*,
*I. Guarneri***, *D.L. Shepelyansky*

Institute of Nuclear Physics
630090, Novosibirsk, USSR

ABSTRACT

We present new data from numerical simulation of microwave excitation of a 2-dimensional Hydrogen atom which show that in a wide parameter range, under the 1-dimensional delocalization border, the quantum localization phenomenon persists. We theoretically reconsider the problem of 2-dimensional localization by using an appropriately constructed 4-dimensional map over an orbital period of the electron, and thus explain the numerical results.

* Permanent address: Dipartimento di Fisica dell'Universita, Milano, Italia.

** Permanent address: Dipartimento di Fisica Teorica e Nucleare dell'Universita, Pavia, Italia.

In Refs [1—3] we reported about our extensive studies of a one-dimensional model for a highly excited Hydrogen atom in a linearly polarized monochromatic microwave field. The most interesting effect which was observed and theoretically explained was the localization of the diffusive excitation under the condition:

$$\varepsilon_0 < \varepsilon_q^{(1)} \approx \frac{\omega_0^{7/6}}{\sqrt{6n_0}}, \qquad (1)$$

where $n_0 \gg 1$ is the initially excited level, $\varepsilon_0 = \varepsilon n_0^4$, $\omega_0 = \omega n_0^3$ are rescaled field strength and frequency, and all physical variables are in atomic units. We also checked the validity of the 1-dimensional model for extended states ($n_2 = 1$, $m = 0$; n_2, m — parabolic and magnetic quantum numbers) by means of a 2-dimensional model [3, Fig. 7c], which made use of a basis of unperturbed eigenfunctions up to $n = 128$. This we theoretically explained [1, 3] by deriving a rough estimate for the 2-dimensional delocalization border:

$$\varepsilon_q^{(2)} \sim \frac{\omega_0^{7/6}}{\sqrt{n_0 n_2}}. \qquad (2)$$

Here we report about preliminary results of the 2-dimensional numerical simulation. We used two values of $\omega_0 = 1.5,\ 2.5$; $0.04 \leqslant \varepsilon_0 \leqslant 0.06$; $n_0 = 66$ and $n_2 \leqslant 30$ (which is about the largest possible value). Since $2d$ computations are much more time consuming we had to restrict our simulation to a relatively short number of field periods $\tau \leqslant 120$. In Fig. 1 we show a typical $2d$ behaviour

for the quantum and the corresponding classical model. From Figs 1,*a*,*c* it is apparent that the quantum motion in n is localized. This is also confirmed by the comparison of quantum and classical distribution functions (Figs 2, 3). In Fig. 2 we show the full distribution $F(n, n_2)$, but a better illustration of localization is provided by Fig. 3, where the distribution integrated over n_2 is plotted versus the number of absorbed photons (which, as shown in Ref. [4], more adequatly exposes the localization). Moreover, the localization length in this as well as in all other cases is satisfactorily described by the 1-dimensional estimate [1, 3].

The relevant fact emerges from these data that the n-motion remains essensially 1-dimensional independently of the n_2 value. Another important feature is that the n_2-motion has a qualitatively different character, namely, it shows no localization (at least in the inspected time interval, Fig. 1,*b*) but still has no impact on the localization occurring for the n-motion. This picture is completely different from the one we assumed when deriving (2).

Attempting to understand these numerical results, we developed a new theoretical approach, which is a 2-dimensional generalization of the theory of Ref. [4]. To this end, we first derived a convenient approximate representation for the 2*d* classical dynamics by means of a 4-dimensional mapping that describes the change, during an orbital electron period, in canonical variables N -- the energy divided by ω, Φ — the conjugate phase, which is just the product of $-\omega$ and time, l — orbital momentum, and ψ — the phase conjugated to l. The phase ψ is the angle between the major axis of the ellipse and the external field. This map is found by integrating the exact Hamiltonian equations of motion over an orbital period. While doing so, we substituted unperturbed motion in the field dependent terms and we kept only the resonant term of the perturbation.

As a result, we found that the generating function of the map leading to the new values $(\bar{N}, \bar{\Phi}, \bar{l}, \bar{\psi})$ is:

$$G(\bar{N}, \Phi, \bar{l}, \psi) = \bar{N}\Phi + \bar{l}\psi - 2\pi(-2\omega\bar{N})^{-1/2} -$$

$$-k[(1-\omega N\bar{l}^{\,2})\cos\Phi\cos\psi - 1.09\omega^{1/3}\bar{l}\,\sin\Phi\sin\psi], \qquad (3)$$

where $k = 0.822\pi\varepsilon/\omega^{5/3}$. In deriving (3), we also assumed $l < \left(\frac{3}{\omega}\right)^{1/3}$ and $\omega n^3 \geqslant 1$. This ensures that the Fourier components of the perturbation decay according to a power law. In order to

simplify the map, it is convenient to go over to new canonical variables (N, θ, J, χ) [5, 6]:

$$\operatorname{tg}\chi = \frac{B}{A}\operatorname{tg}\psi, \quad \theta = \Phi + \chi,$$

$$J + N = \int_0^l \frac{AB\,dl'}{A^2\sin^2\chi + B^2\cos^2\chi}, \qquad (4)$$

$$A = 1 - Nl^2\omega, \quad B = 1.09\,\omega^{1/3}l.$$

In these new variables the map is given by:

$$\bar{J} = J + k\frac{\partial H}{\partial\chi}\cos\theta,$$

$$\bar{\chi} = \chi - k\frac{\partial H}{\partial\bar{J}}\cos\theta,$$

$$\bar{N} = N - kH\sin\theta, \qquad (5)$$

$$\bar{\theta} = \theta - 2\pi\omega(-2\omega\bar{N})^{-3/2} - k\frac{\partial H}{\partial\bar{N}}\cos\theta,$$

where $H^2(N, J, \chi) = A^2\cos^2\psi + B^2\sin^2\psi$. Under appropriate conditions to be specified below, it is possible to neglect the dependence of H on N, and to use a continuous time approximation for (J, χ) equations. Then, introducing a new time σ defined by $\frac{d\sigma}{dt} = k\cos\theta$ (t is the number of iterations) the (J, χ) continuous-time dynamics will be ruled by the Hamiltonian H, which is a constant of the motion. In this case, the (N, θ) motion will be strictly 1-dimensional. For approximately 1-dimensional states ($l \ll n$, $\psi \ll 1$), $H \approx 1$ and the (N, θ) equations coincide with the 1-dimensional equations [4]. Anyway, even for more general states, we shall obtain a 1*d* situation in the (N, θ) equations (5), with kH in place of k. As to the (J, χ) dynamics, in the new time σ it will not depend on the (N, θ) motion.

Consider a case in which a regular (N, θ) motion is taking place with $\lambda = \cos\theta \neq 0$, then $\sigma = k\lambda t$. This may happen also above the chaotic threshold inside a stable region [3]. For extended states the Hamiltonian H can be approximately written, in the old variables, as:

$$H=1+\frac{1}{2}\left(\frac{l^2}{n^2}-\psi^2\right) \qquad (6)$$

with n constant. The motion described by (6) is unstable, with a characteristic instability time $\sigma_r=n$ or $t_r=\frac{n}{k\lambda}$, as was pointed out in [6]. Nevertheless, the long-term motion is certainly periodic, with a period $T_r\sim 2t_r\Lambda$ and $\Lambda\sim \ln\frac{n}{n_2}$. Thus, one condition for the continuous-time approximation to hold is $t_r\approx\frac{\omega_0^{5/3}}{2.6\,\varepsilon_0\lambda}\gg 1$. In the opposite case of a completely chaotic (N,θ) motion, $\sigma(t)$ is a random function with $\overline{\sigma(t)}=0$, $\overline{\sigma^2(t)}=\frac{k^2t}{2}$. Then the average of the exponent σ/n in the solution of (6) is given by $\overline{\left(\frac{\sigma}{n}\right)^2}=\frac{k^2t}{2n^2}$. Whence we see that the characteristic time of the motion is now $t_{ch}=2\left(\frac{n}{k}\right)^2\gg t_r$. This time can be compared with the ionization time $t_l\approx\frac{2N_0^2}{k^2}$, where $N_0=-\frac{1}{2n_0^2\omega}$, finding that $t_{ch}/t_l\approx 4\omega_0^2\gg 1$.

If the Hamiltonian (6) is written in the variables N, l, ψ $\left(N=-\frac{1}{2n^2\omega}\right)$ the approximate equation $\delta H\sim\omega l^2\delta N$ is gotten, and a condition under which the N-dependence of H can be neglected takes the form: $\omega l^2\delta N\ll\left(\frac{l}{n}\right)^2\ll 1$

In the quantum case, in this approximation of constant H, we get the usual 1-dimensional localization for the N-motion with the localization length $\mathscr{L}\approx\frac{k^2}{2}H^2\approx\frac{k^2}{2}$, independently of the (l,ψ) dynamics. This explains the behaviour observed in the above described numerical results (Figs 1—3). In these results, the n_2-motion has a regular character in spite of the chaotic (N,θ) motion. On the one hand, the chaotic time scale $\tau_{ch}=\omega_0 t_{ch}\sim 10^4$ for the parameter values of Figs 1—3, so that the diffusion in n_2 could not be detected in the actual time of observation. On the other hand, for the used value of ε_0 stable regions in the (N,θ) motion are known to exist, which are apparently responsible for the observed regular behaviour of n_2. Using the explicit solution for the motion described by (6), and the relation

$$\frac{n_1-n_2}{n}=\sqrt{1-\frac{l^2}{n^2}}\cos\psi,$$

which approximately gives $n_2\approx\frac{1}{4}\left(\frac{l^2}{n}+n\psi^2\right)$, we get

$$n_2\approx n_{20}\left[\mathrm{ch}\left(\frac{2\sigma}{n}\right)+\sin 2\eta_0\,\mathrm{sh}\left(\frac{2\sigma}{n}\right)\right]. \qquad (7)$$

Here η_0 is the initial value of the phase conjugated to n_2, which must be assumed to be uniformly distributed in $(0,2\pi)$ in order to reproduce the initial quantum state. From (7), by phase averaging, we find the dependence of the first two moments of n_2 on the time σ:

$$\mu_1=\langle n_2-n_{20}\rangle=n_{20}\left(\mathrm{ch}\frac{2\sigma}{n}-1\right),$$

$$\mu_2=\langle(n_2-\langle n_2\rangle)^2\rangle=\frac{n_{20}^2}{2}\,\mathrm{sh}^2\frac{2\sigma}{n}. \qquad (8)$$

For $\frac{2\sigma}{n}\ll 1$ the ratio $\frac{\mu_2}{\mu_1}\approx n_{20}$, which reasonably agrees with numerical data (Fig. 1,*b*). From the comparison of (8) with numerical data we can calculate the regular characteristic time: $\tau_r\approx 2800$ in the classical case and $\tau_r\approx 3600$ in the quantum case. Then we can also find the corresponding values of the factor λ which relates the values of the times τ and σ : $\lambda\approx 0.04$ and $\lambda\approx 0.03$. These relatively small values of $\lambda=\cos\theta$ may be related to the fact that the value of $\omega_0=2.5$ lies just between two main resonances, so that the stable region is relatively small for the chosen initial conditions. Hence the instability in the n_2-motion is very slow [3]. We think that the difference between the quantum and the classical values of λ can be explained by the fact that, due to interference, the small regular component of the motion has, in the quantum case, a different interaction with the chaotic one.

The next important question is what would be the impact of a small change in H on the (N,θ) dynamics and whether, in particular, it could lead to 2-dimensional delocalization. We think that the latter could not happen, unless t_{ch} becomes comparable with the localization time $\sim\mathscr{L}$. Indeed, the (l,ψ) motion would just broaden

the lines in the discrete spectrum of the (N, θ) motion, up to the width $\sim 1/t_{ch}$. In order to provide delocalization it is at least necessary (but perhaps not yet sufficient) that $t_{ch}^{-1} > \mathscr{L}^{-1}$ (the average spacing in the discrete spectrum), or $\mathscr{L} > t_{ch}$. This cannot happen below the 1-dimensional delocalization border because the ratio $t_{ch}/\mathscr{L} \sim (\varepsilon_q^{(1)}/\varepsilon_0)^4 \omega_0^2 \gtrsim 1$. Another way to put it is that the slow (l, ψ) motion acts as an adiabatic perturbation on the (N, θ) motion, which cannot produce any additional transitions in the latter. The ultimate origin of this adiabaticity is the Coulomb degeneracy.

Therefore it appears that in order any truly 2-dimensional delocalization may occur the approximate conservation of H must be destroyed, and a sufficiently short time scale for the (l, ψ) motion must be provided. This is why our previous estimate (2) failed: indeed, in deriving it both these conditions were implicitly assumed. We conjecture, and are currently investigating, that 2-dimensional delocalization can be achieved by introducing a relatively strong static field. Without static field the localization of diffusive excitation appears as typical a phenomenon in the 2-dimensional case as it was found to be in the 1-dimensional case.

REFERENCES

1. *G. Casati, B.V. Chirikov, D.L. Shepelyansky*, Phys. Rev. Lett. 53 (1984), 2525.
2. *G. Casati, B.V. Chirikov, I. Guarneri, D.L. Shepelyansky*, Phys. Rev. Lett., 57 (1986), 823.
3. *G. Casati, B.V. Chirikov, I. Guarneri, D.L. Shepelyansky*, Preprint, Milano University, 1986.
4. *G. Casati, I. Guarneri, D.L. Shepelyansky*, Preprint INP 87-29, Novosibirsk 1987.
5. *B.I. Meerson, E.A. Oks, P.V. Sasorov*, J. Phys. B, 15 (1982), 3599.
6. *J.G. Leopold, D. Richards*, J. Phys. B, 19 (1986), 1125.

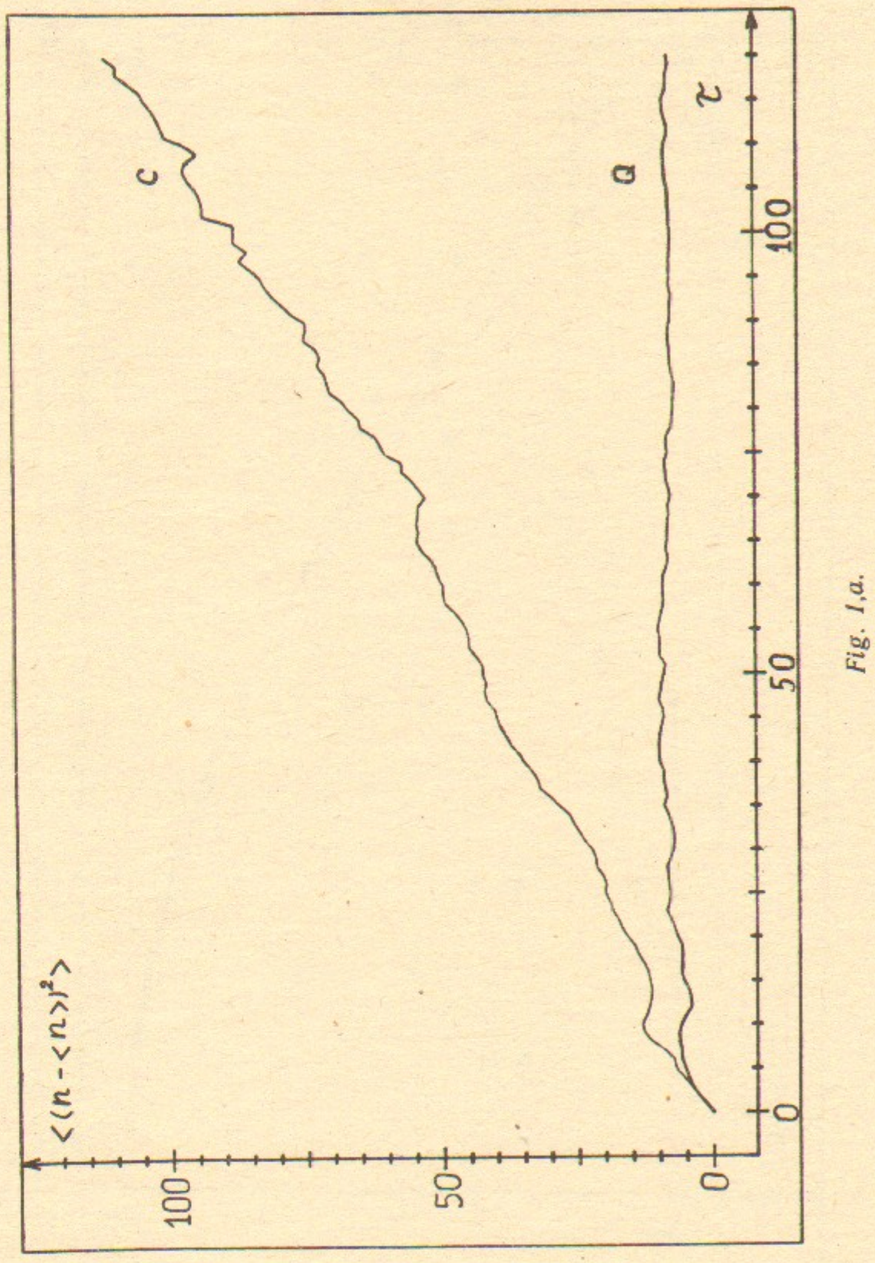

Fig. 1,a.

Fig. 1. Time dependence, in the quantum (Q) and classical (C)·2-dimensional models, of the second moment μ_2 for n (a); of μ_2 for n_2 (lines—left scale) and of the ratio $\mu_2/\mu_1 n_{20}$, where μ_1 is the first moment for n_2 (dots and circles—right scale) (b); and of the probability excitation $W_{1.5}$ above $n \approx 1.5 n_0$ (quantum values are multiplied by 100) (c). The parameter values are: $n_0 = 66$, $\omega_0 = 2.5$, $\varepsilon_0 = 0.04$, $n_{20} = 15$; τ is the number of field periods.

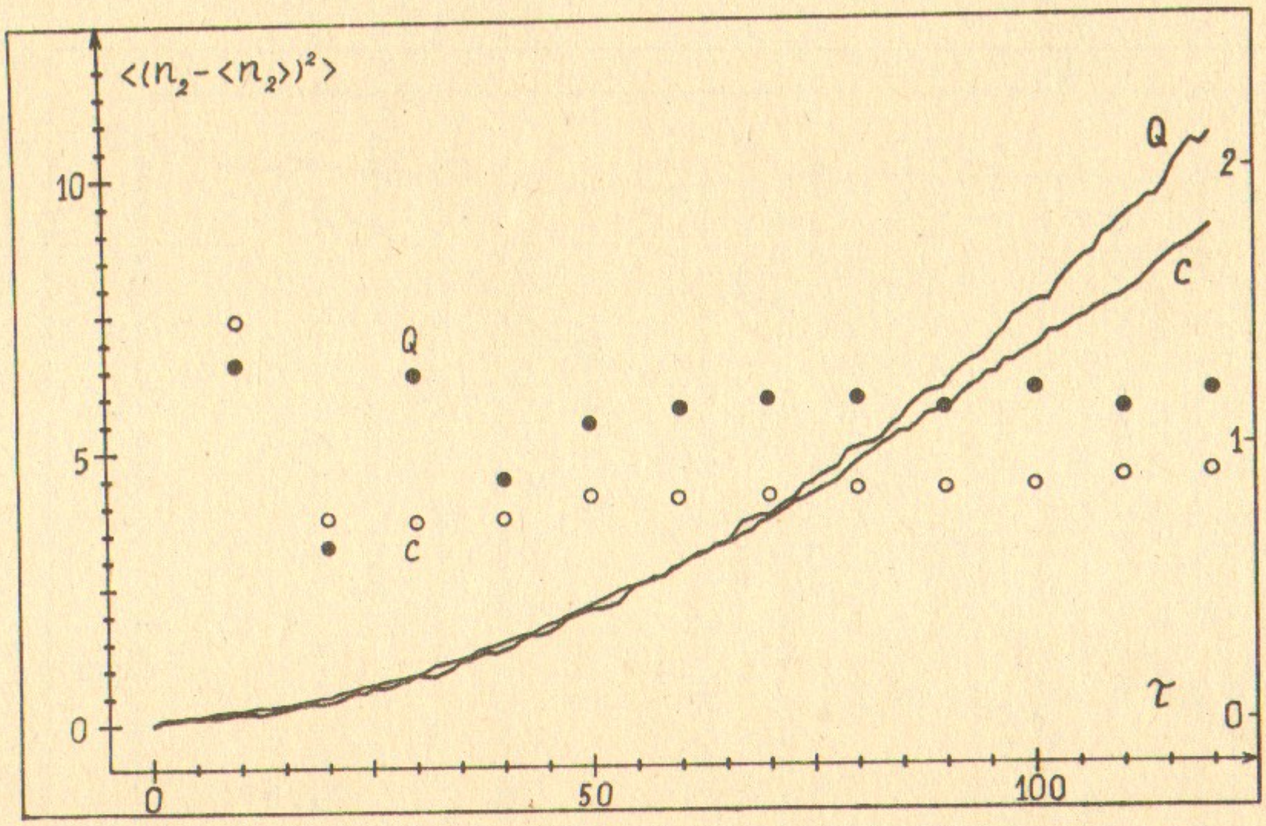
$\langle (n_2 - \langle n_2 \rangle)^2 \rangle$
10
5
0
Q
C
Q
C
2
1
0
τ
0
50
100

Fig 1,b.

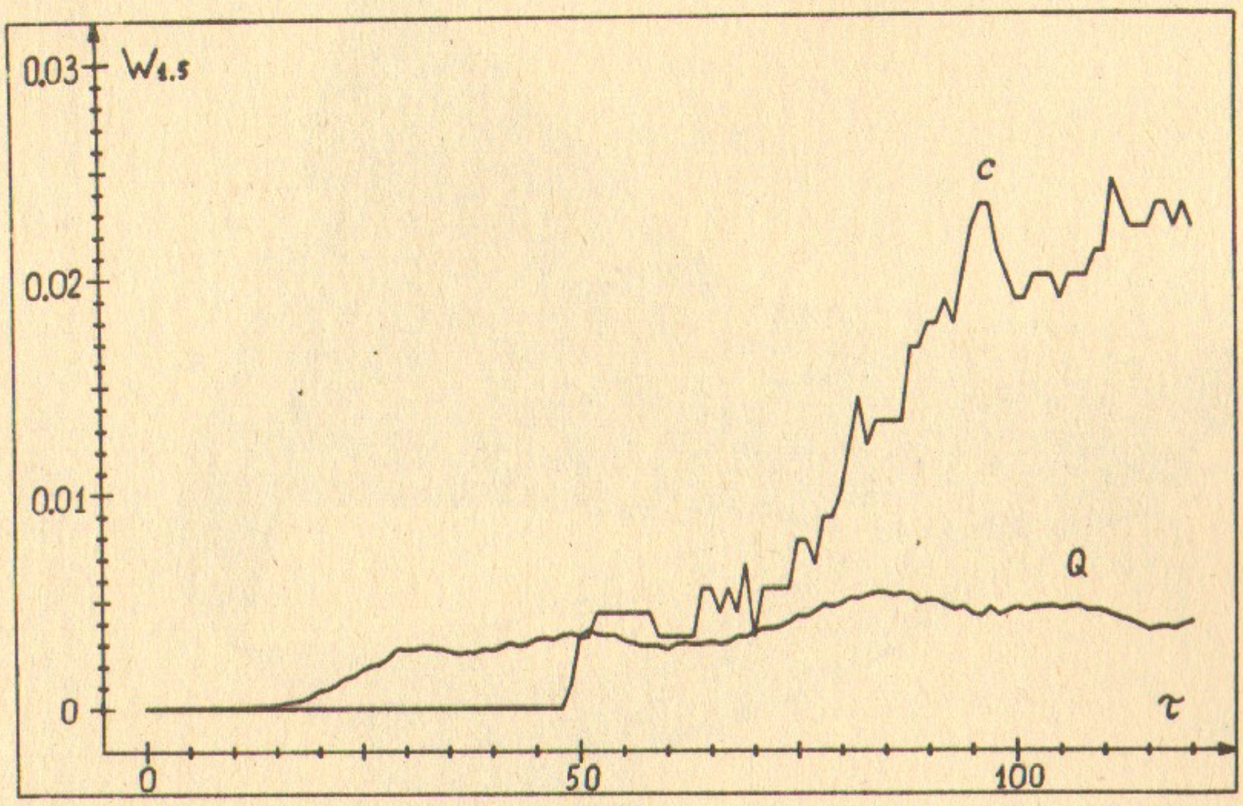
0.03
$W_{4.5}$
0.02
0.01
0
C
Q
τ
0
50
100

Fig.1,c.

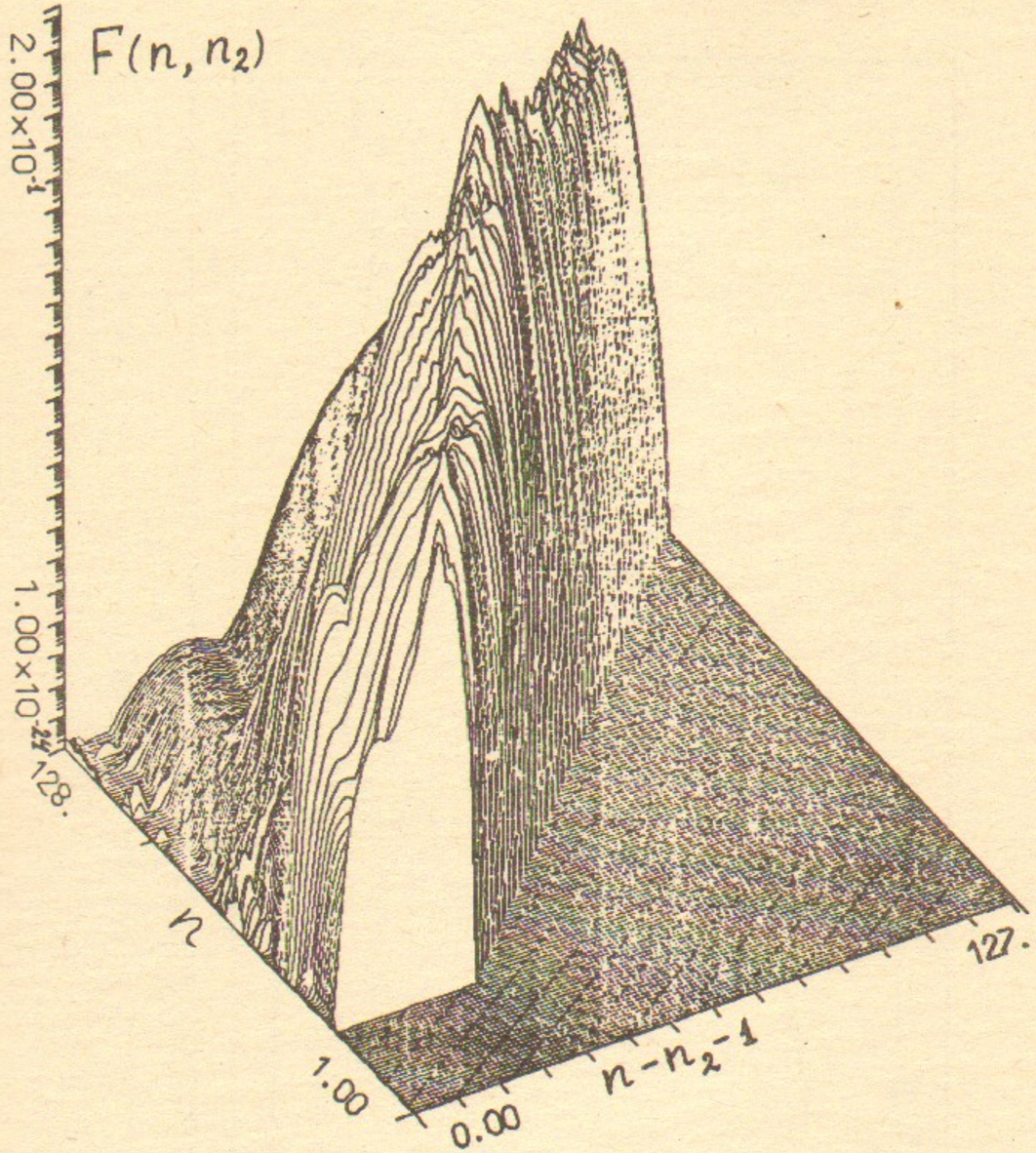

Fig. 2. An example of the full distribution $F(n, n_2)$ for the same parameter values as in Figs 1, 3.

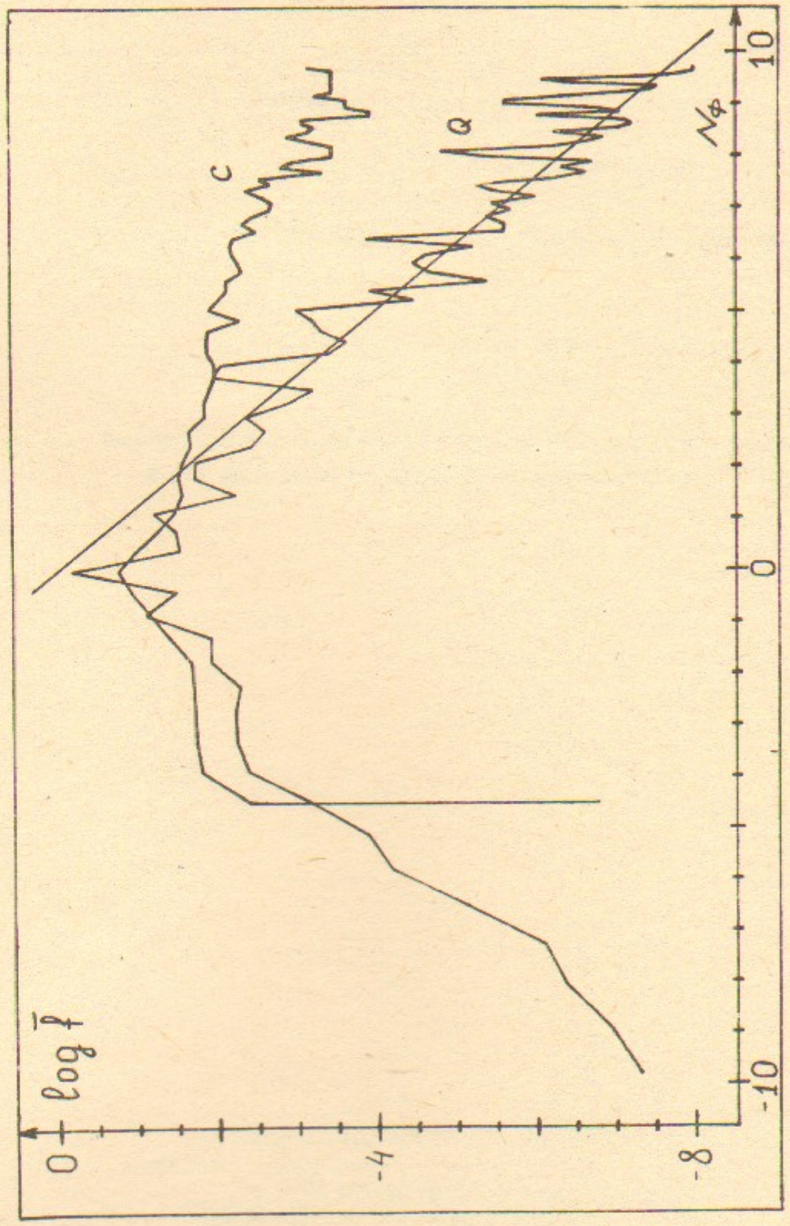

Fig. 3. Classacal (C) and quantum (Q) distribution functions versus the number of absorbed photons $N_\Phi = \left(\frac{1}{2n_0^2} - \frac{1}{2n^2}\right)/\omega$ [4] averaged in time from $\tau = 110$ to $\tau = 120$. The straight line is the 1-dimensional theoretical exponential distribution, and the parameter values are as in Fig. 1.

G. Casati, B.V. Chirikov,
I. Guarneri, D.L. Shepelyansky

Two-Dimensional Localization of Diffusive Excitation in the Hydrogen Atom in a Monochromatic Field

Дж. Казати, Б.В. Чириков, И. Гварнери,
Д.Л. Шепелянский

Двумерная локализация диффузионного возбуждения для атома водорода в монохроматическом поле

Ответственный за выпуск С.Г.Попов

Работа поступила 18 февраля 1987 г.
Подписано в печать 25.03 1987 г. МН 08661
Формат бумаги 60×90 1/16 Объем 1,0 печ.л., 0,9 уч.-изд.л.
Тираж 290 экз. Бесплатно. Заказ № 30

Набрано в автоматизированной системе на базе фотонаборного автомата ФА1000 и ЭВМ «Электроника» и отпечатано на ротапринте Института ядерной физики СО АН СССР,
Новосибирск, 630090, пр. академика Лаврентьева, 11.