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ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

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PREPRINT 84-144

НОВОСИБИРСК

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A b s t r a c t

We numerically study the excitation mechanism of the hydrogen atom in a microwave field and show that quantum mechanics imposes limitations to the classical chaotic motion. Besides, a multiphoton resonance pattern has been found. We suggest that a direct laboratory experimental verification of these phenomena should be possible.

To explain the results of experiments[1,2] on ionization of highly-excited hydrogen atoms by a microwave monochromatic field, a new mechanism of ionization has been suggested[3], namely, a quantum diffusion of the electron over the unperturbed excited states. Since in actual experiments only initial states corresponding to high values of the principal quantum number ($n = 45$-66) were examined, a classical description of the problem was given[4] and the numerical results obtained were in satisfactory agreement with experiments in Ref. (1). In Ref. (5) the essential role of classical chaotic motion was stressed and the condition for the onset of diffusive behavior has been derived. However, the numerical experiments with simple quantum models[6-9] have shown that the quantum effects lead to the limitation of classical chaotic excitation. Also, computer simulations of the electron excitation from extended states, i.e. states with parabolic quantum numbers $n_1 \gg n_2 \sim 1$ (or $n_1 \ll n_2$), have revealed that diffusion over levels is much slower in the quantum case than in the classical[10]. Moreover, besides the diffusion, multiphoton resonances with the number of photons $k \sim 10$ were found to play a significant role in the excitation,

This paper is devoted to a numerical study of the dynamics of the hydrogen atom excitation from states with $n_1 \gg n_2 \sim 1$ and $m = 0$. As these states are very extended along the field direction we make use of the one-dimensional model developed and described in detail in Ref. (10). The Hamilton operator of the model is*)

$$\hat{H} = \frac{\hat{p}_z^2}{2} - \frac{1}{|z|} + \varepsilon z \cos \omega t \qquad (1)$$

where ε , ω are the field strength and frequency in atomic units. In our computations we used initial conditions corresponding to a single excited unperturbed level with $n_0 = 45$, 56 or 66. The total number of levels taken into account was about 200 in a typical range $20 \leq n \leq 226$.

The accuracy of the numerical results was checked by varying the total numbers of levels. For comparison we integrated the classical equations of motion for 250 trajectories with

*) In the classical limit this model was first considered by R.V.Jensen Ref. (11,12) for the description of a different physical system, the so-called surface-state electrons.

the same initial value of the action n_o and phases homogeneously distributed over the interval $[0,2\pi]$. The main computations have been carried out on a CRAY-1S computer.

The quantum limitation on chaotic excitation was one of the most interesting phenomena observed in our numerical experiments. Consider, for example, a typical case with $n_o = 66$, $\omega_o = \omega n_o^3 = 1.2$ and $\varepsilon_o = \varepsilon n_o^4 = 0.03$. Here, in the classical limit, the resonance overlap condition is fulfilled which leads to a diffusive excitation of the electron(13). In order to investigate the extent to which diffusion also occurs in the quantum case we considered the second moment $M_2 = \langle (n-\langle n\rangle)^2 \rangle / n_o^2 \equiv \langle (\Delta n)^2 \rangle / n_o^2$ of the distribution function f_n over the energy levels. We found that in the quantum case the dependence of M_2 on the time is qualitatively different from that in the classical limit. Indeed, the quantum moment M_2 remains close to the classical one during a few periods of the field only, and then it oscillates about a stationary value whereas the classical moment continues to grow rapidly (Fig. 1). This confirms the previous results of Ref. (10). Increasing the peak value of the field to $\varepsilon_o = 0.04$ leads to a sharp rise in the quantum moment M_2 which continues during the whole computation time. However, the growth rate is definitely smaller than in the classical case (Fig. 1). Similar phenomena were also observed for different values of the parameters, for example, at $\omega_o \approx 1$; $n_o = 66$, $\varepsilon_o = 0.03-0.04$ and $n_o = 45$, $\varepsilon_o = 0.04-0.05$.

To get some insight into the nature and mechanism of the sharp increase in M_2 with ε_o (Fig. 1) we turned to the distribution function $f_n(\tau)$ where $\tau = \omega t/2\pi$. An example of $\bar{f}_n$ averaged (to suppress the fluctuations) over the 40 values in the interval $80 < \tau \leq 120$ for the case $\varepsilon_o = 0.03$ of Fig. 1 is shown in Fig. 2. Most of the probability is concentrated within a peak whose maximum remains at the initial level $n = n_o$ in all cases. Even though the moment M_2 keeps growing, the width of the peak increases only up to a stationary value. Such a behavior corresponds to the so-called quantum localization in a classicaly chaotic system which was studied in the simple rotator model(6-9,14) and then confirmed in other models(15,16) as well. The peak shape can be approximately described by the

simple exponential dependence

$$f_n \propto \exp\left(-\frac{2|n-n_o|}{\ell}\right) \tag{2}$$

in agreement with the results obtained for the rotator model(9,17). The order of magnitude of the localization length ℓ can be estimated by the simple method described in Section 3.4 of Ref. (7) which gives

$$\ell \approx \alpha D_{cl} \equiv \alpha \frac{d}{d\tau}\langle(\Delta n)^2\rangle = \alpha n_o^2 \frac{dM_2}{d\tau} \tag{3}$$

The factor α is close to one according to numerical data on the rotator model (see(9,17)).

Eq. (3) holds for homogeneous diffusion only ($D_{cl} \approx$ const). However the diffusion coefficient for the model (1) in the quasilinear approximation depends on n(13):

$$D_{cl} \approx \frac{2\varepsilon_o^2 n^3}{\omega_o^{7/3} n_o} \tag{4}$$

(This expression has also been verified in Ref. 12). Nevertheless for sufficiently small ε_o, ℓ is also small and $n \approx n_o$ so Eq. (3) still holds. Yet, for large ε_o, n grows rapidly which leads to delocalization, and to unlimited diffusion with a rate close to the classical one. This phenomenon was investigated and explained for a simple model(7).

The analytical expression for the dependence of localization length on the parameters can be derived also in the present case and has the following form (the related theory will be published elsewhere):

$$\ell \approx 0.4 \frac{\omega_o^{7/3}}{\varepsilon_o^2} u \tag{5a}$$

where u is smaller of the two solutions to the equation

$$\frac{\omega_o^{14/3}}{\mathcal{E}_o^4 n_o^2} = \frac{9}{4} \frac{(2-u)}{u(1-u)^2} \qquad (0 < u < 1) \qquad (5b)$$

For

$$\mathcal{E}_o \gtrsim \frac{\omega_o^{7/6}}{2\sqrt{n_o}} = \mathcal{E}_q^{(1)} \qquad (6)$$

Eq, (5b) has no solution which means delocalization, i.e. indefinite diffusion, and $\mathcal{E}_q^{(1)}$ is the <u>quantum delocalization border</u>. Of course, this holds if $\mathcal{E}_o$ exceeds also the classical chaos border[13] $\mathcal{E}_c \approx \frac{1}{50} \omega_o^{-1/3}$. Notice that the critical value (6) corresponds to the condition $\ell \sim n_o$ with ℓ given by Eq. (3). Indeed, for $\ell > n_o$ the increase in the diffusion coefficient with n needs to be taken into account. In Fig. 3 the analytical expression (5) is compared with numerical data obtained in the present work. The rather big scattering of points about the theoretical curve may be explained, at least partially, by the regions of stable classical motion which still survive for the given values of the parameters.

The observed fast growth of the moment M_2 in Fig. 1 cannot be explained by the phenomenon of delocalization since the corresponding values of $\mathcal{E}_o$ are subcritical. Instead, it is apparently related to the broad multiphoton "plateau" in the distribution function (Fig. 2). This plateau has an evident resonance structure. The spacings in the unperturbed energy between principal peaks are approximately equal to the frequency of the external field. Twelve such peaks, equally-spaced in energy, are fairly clear in Fig. 2. In some cases several series of equally-spaced peaks were observed: for example, at n_o = = 56, ω_o= 0.8, $\mathcal{E}_o$= 0.03 there are three such series.

The total probability of states within the plateau can be roughly estimated by the excitation probability $W_{1.5}$ into the states with $n \geqslant [1.5 n_o]$ where brackets denote the integer part. The increase in $\mathcal{E}_o$ from 0.03 to 0.04 changes this probability, at τ = 80, from $4.1 \cdot 10^{-4}$ to $3.6 \cdot 10^{-2}$ and enhances the multiphoton plateau by two orders of magnitude which explains the

sharp growth of M_2 in Fig. 1. The field dependence of excitation probability can be approximately described by the empirical power law $W_{1.5} = (\mathcal{E}_o/\mathcal{E}_a)^{2k_E}$ with $k_E \approx 7.8$ and $\mathcal{E}_a \approx 0.05$. This k_E value is considerably smaller than the number of photons required for the direct transition from n_o to $n \approx 1.5\, n_o$ which is approximately equal to $k_D = [5n_o/18\omega_o] + 1 = 16$. Similarly, for $n_o = 45$, $\omega_o = 1$ the quantities $k_E \approx 3.9$, $\mathcal{E}_a \approx 0.063$, $k_D = 13$, and for $n_o = 66$, $\omega_o = 1$ they are $k_E \approx 7.8$, $\mathcal{E}_a \approx 0.045$, $k_D = 19$.

The results obtained here suggest the following qualitative cascade picture of the atom excitation. First, the initial state is spreading (Fig. 1) until the localization width ℓ is reached (see Fig. 3 and Eq. (5)). Then one or a few multiphoton transitions (their number determines the number of equally-spaced series) transfer the localized excitation onto the higher levels. Here the field is strong enough to provide one-photon transitions with a high probability and this results in the appearance of a series of equidistant peaks (Fig. 2).

It is interesting to note that no multiphoton effects were observed in the rotator model[6,7] (for irrational $T/4\pi$). This is apparently related to a different structure of the unperturbed spectrum as well as to analiticity of the perturbation which implies an exponential decrease in its matrix elements. We note that the harmonic time dependence of the perturbation in (1) is important; for example, replacement of the latter with a delta-function [16] may qualitatively change the multiphoton processes. The role of the latter in another model was also discussed in[15].

The one-dimensional model investigated here does not take into account the change in the second quantum number n_2. As shown in Ref. (10) the matrix element related to the transition with $\Delta n_2 = 1$ is smaller than that for $\Delta n_1 = 1$ by a factor of n_2/n, and the corresponding probability is $(n_2/n)^2$ times less, while the frequencies in both cases are approximately the same, due to the Coulomb degeneration. Therefore, as long as $n_2 \ll n$ the influence of the second dimension on the multiphoton transitions appears to be small. Yet, its impact on the quantum limitation of diffusion may be significant.

Indeed, as in the stochastic region n_2 is diffusing at the rate $D_{n_2} \approx D_{cl} \left(\frac{n_2}{n}\right)^2$ (10), the number of excited levels is $N = \doteq \Delta n_1 \cdot \Delta n_2 \sim D_{cl} \frac{n_2}{n} \tau$ $(n_2 \neq 0)$. According to Ref. (7,14,10) the condition for delocalization is then $N \gtrsim \tau$. Hence, from (4) the two-dimensional delocalization border is at:

$$\varepsilon_0 \sim \varepsilon_q^{(2)} = \frac{\omega_0^{7/6}}{\sqrt{n_2 n_0}} \qquad (7)$$

Thus, the second dimension sharply decreases the delocalization border. For $n_2 \sim n_0$ and $\omega_0 \sim 1$ the critical value $\varepsilon_q^{(2)} \sim 1/n_0$ which, for $n_0 \sim 60$, is approximately equal to the classical chaos border. This may explain the agreement with experiments of the classical computations in Ref. (4). However, for $n_2 \sim 1$ the border (7) is of the same order as in the one-dimensional case (6). Therefore one may expect that for extended states ($n_2 \sim 1$) and for a smaller field than (6) the localization will persists in the two-dimensional case as well and can be observed experimentally.

Another effect omitted in our numerical experiments is transitions to continuous spectrum. An indirect check of the importance of this process can be obtained as follows. The numerical code used here causes a decrease in normalization W at a rate proportional to $(\varepsilon n^2 \Delta t)^6$, where $\Delta t = 2\pi/\omega L$ is the integration time step and L is the number of steps per period of the external field. This "artificial damping" results in a stationary probability flow in regions of high n values. We have found that even for strong fields (for example, $\varepsilon_0 = 0.05$, $\omega_0 = 1$, $n_0 = 45$, $L = 800$, $n_{max} = 211$) this flow is fairly small ($\frac{dW}{d\tau} \approx 4 \cdot 10^{-5}$), and does not affect the distribution f_n. This suggests that for a low multiphoton plateau the transitions into continuous spectrum would not change the whole excitation significantly.

Acknowledgements. We are greatly indebted to I.Guarneri, F.Vivaldi, J.Ford and F.Izrailev for simulating discussions and useful suggestions.

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Figure captions

Fig. 1. Dependence of the second moment $M_2 = \frac{\langle(n-\langle n\rangle)^2\rangle}{n_0^2}$ on time $\tau = \frac{\omega t}{2\pi}$ measured in the number of field periods. Quantum case: $n_0 = 66$, $\omega_0 = 1.2$; $\varepsilon_0 = 0.03$ (curve 1), $\varepsilon_0 = 0.04$ (curve 3). Curves 2 and 4 correspond to the classical limit of 1 and 3 respectively.

Fig. 2. Distribution function $\bar{f}_n$ averaged over 40 values within the interval $80 < \tau \leq 120$ for the quantum case 1 of Fig. 1 (full line) and for the classical case 2 of Fig. 1(dashed line); n_c is the classical chaos border. Arrows are drawn with equal spacing $\Delta E = \omega$ (in energy scale), one arrow being attached to the empirical peak at n = 142.

Fig. 3. Dependence of the localization length ℓ on the model parameters in log-log scale. The solid curve corresponds to the theoretical expression (5); points are calculated from numerical data; the vertical dashed line shows the quantum delocalization border (6).

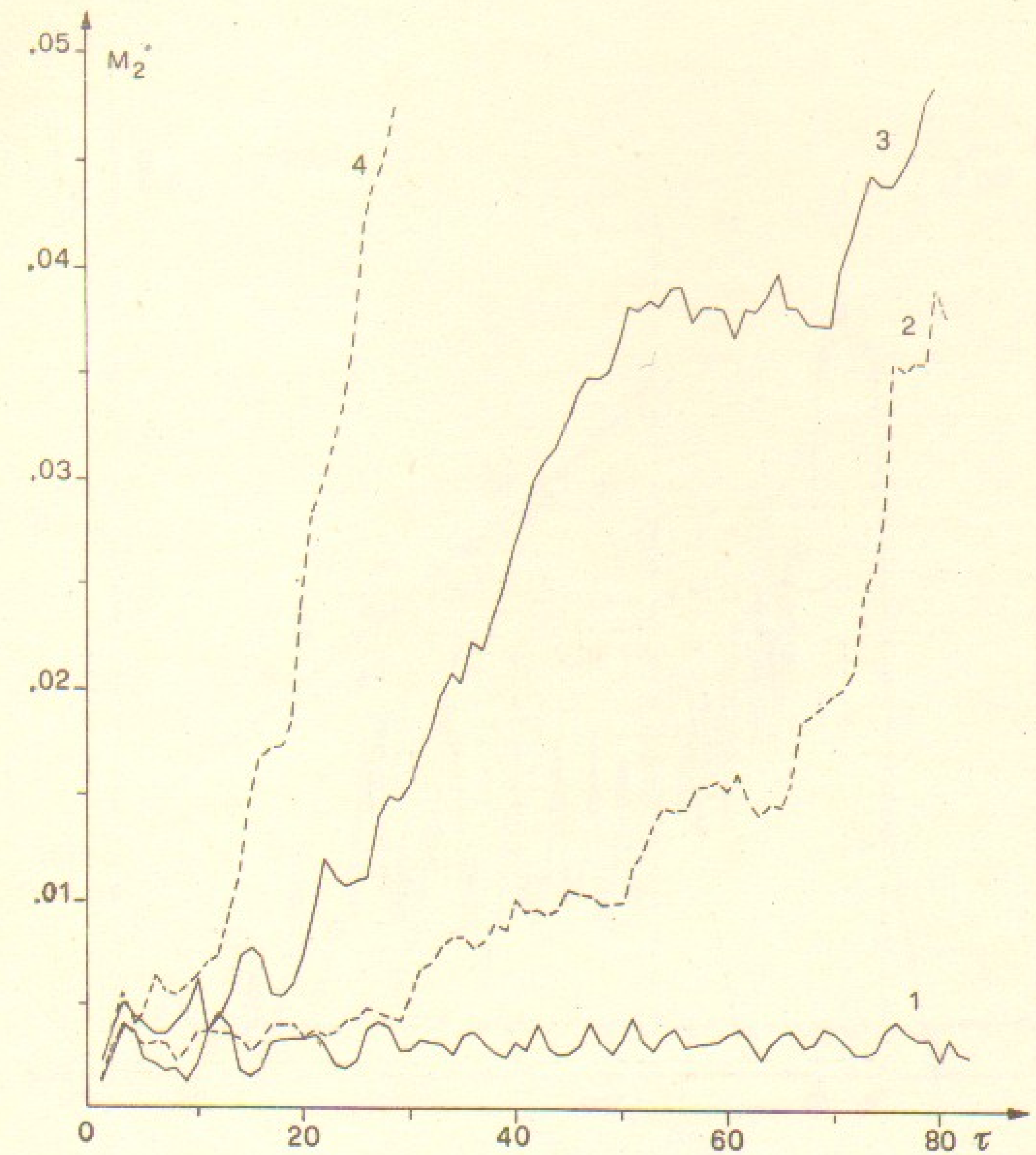

Fig. 1.

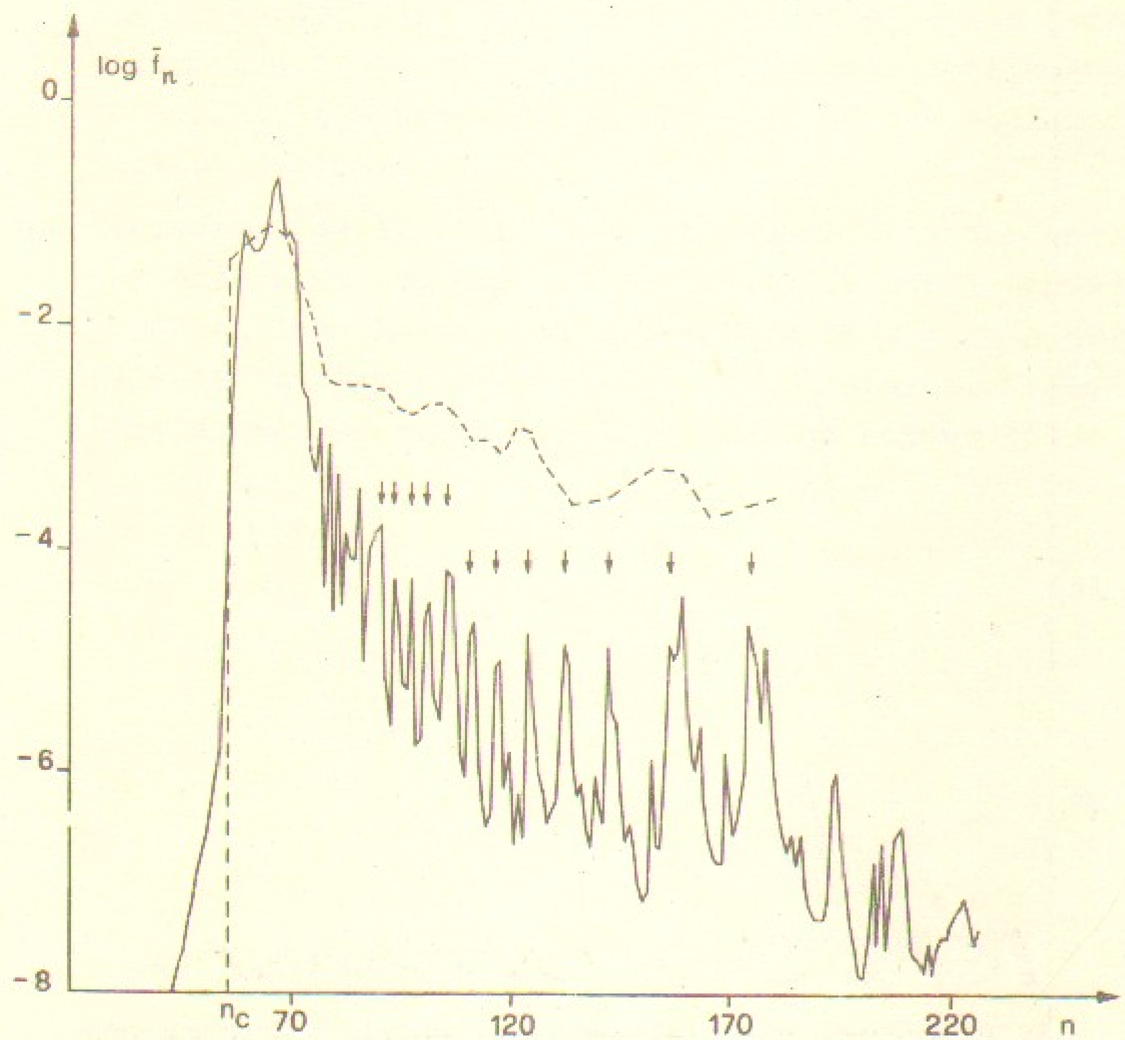
log f̄n
0
-2
-4
-6
-8
nc
70
120
170
220
n

Fig. 2.

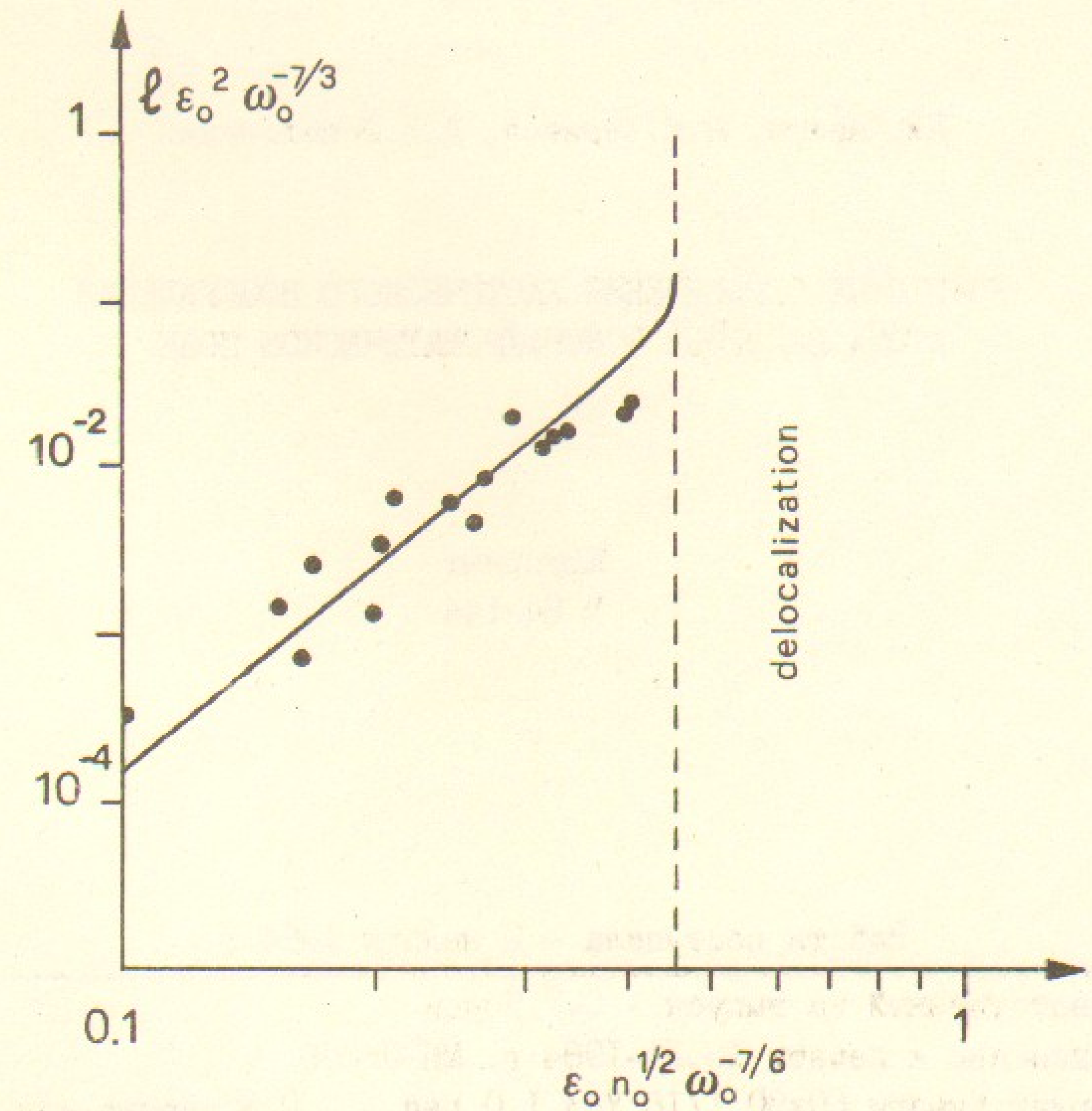
ℓ ε₀² ω₀^{-7/3}
1
10^{-2}
10^{-4}
delocalization
0.1
1
ε₀ n₀^{1/2} ω₀^{-7/6}

Fig. 3.

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

КВАНТОВЫЕ ОГРАНИЧЕНИЯ ХАОТИЧЕСКОГО ВОЗБУЖДЕНИЯ
АТОМА ВОДОРОДА В МОНОХРОМАТИЧЕСКОМ ПОЛЕ

Препринт
№ 84-I44

Работа поступила - 2 ноября I984 г.

Ответственный за выпуск - С.Г.Попов
Подписано к печати I2.XI-I984 г. МН 06208
Формат бумаги 60х90 I/I6 Усл.I,0 печ.л., 0,9 учетно-изд.л.
Тираж 290 экз. Бесплатно. Заказ № I44.

Ротапринт ИЯФ СО АН СССР, г.Новосибирск, 90