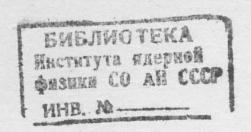


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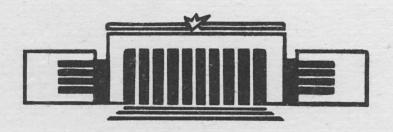
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BEHAVIOR OF HYDROGEN ATOM UNDER THE INFLUENCE OF PERIODIC TIME-DEPENDENT ELECTRIC FIELDS



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НОВОСИБИРСК

BEHAVIOR OF HYDROGEN ATOM UNDER THE INFLUENCE OF PERIODIC TIME-DEPENDENT ELECTRIC FIELDS

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Abstract

The behavior of a hydrogen atom under the influence of periodic impulsive electric fields is studied. The dynamics of excited states are examined both for weak and strong fields. The results differ from the corresponding classical predictions even when n >> 1. In the quantum calculations, the ionization is caused by direct coupling to the ionization channels while the initial probability distribution remains highly localized. There is suppression of "classical stochastic diffusion" over the discrete states, even for relatively strong external field strengths. The numerical method adopted can be used for fields with an arbitrary time-dependence.

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I. INTRODUCTION

In recent years, attention^{1,2} has been paid to the study of the behaviour of highly-excited atoms in intensive external electromagnetic fields. One of the most interesting and important questions concerns the mechanism and condition for the ionization of such atoms in external fields of frequency less than ionization threshold. In such cases the nonlinear effects of the field-atom interaction become very important³. To date, field-atom interactions have generally been studied³⁻⁵ for cases where the atoms populated low-excited states.

However, for field-atom interactions involving atoms in highly-excited states, the usual perturbative approach is not valid. Moreover, for large n (\gg 1), effects can arise which have no analogy to the cases with small n(\geqslant 1). On the other hand the experimental situation is also complicated by the necessary to first populate the high Rydberg states. Nevertheless, experimental data^{6,7} on the ionization of the hydrogen atom in an initial state with n_o \sim 45; 66 are available.

As is known from the general theory of ionization of atoms, that for a short ranged potential, the nature of the nonlinear ionization is determined by an adiabaticity parameter⁸:

 $\chi = \frac{\omega}{nE}$

where ω and ξ are respectively the frequency and strength of the electric field and n is the principal quantum number of the level under consideration. It is generally considered that $\chi^2 \gg 1$ for a multi-photon ionization, while for ionization caused by tunnelling, $\chi^2 \ll 1$. For atoms in highly excited states, such conditions have been studied recently. The critical value of χ for the Keplerian frequency $\omega \approx 1/n^3$ has been found to be $\chi_{cr} \approx 7$.

However, for large $n \gg 1$, it has been suggested ¹⁰ that ionization can also be caused by stochastic diffusion. This results in a diffusive excitation of higher levels up to the continuum. For the hydrogen atom in a circular polarized monochromatic field, various analytical estimates based on the criterion of overlapping nonlinear resonances ^{12,13} have been

derived 11, from which it is possible to indicate a measure of the critical field above which the stochastic diffusion in the hydrogen atom is likely to occur. These estimates have, however, been further refined and generalized 2, 14.

The experimental feasibility of the study of ionization of highly excited hydrogen atoms has stimulated a large number of numerical calculations 15,17 based on semi-classical descriptions. The results of the calculations have demonstrated with the data, and with the analytical estimates 2,11. It has been shown that for highly excited atoms, besides the multi-photon and tunnel ionization, the classical stochastic diffusion plays an essential (and sometimes, major) role in the ionization process.

According to refs. [2,11], the critical fields for the occurance of stochastic diffusion are determined from the estimate

$$\xi > \xi_{\rm cr} \approx \frac{1}{c n^4} \tag{1.2}$$

where the parameter c ranges between

depending on the orbital quantum number ℓ and on the type of polarization of the monochromatic field. The condition eq. (1.2) is satisfied when the field frequency of the electron and when the field is strong enough. From eqs. (1.1) and (1.2) it follows that the ionization due to tunnelling can be neglected and only the multiphoton ionization can be compared with the stochastic ionization.

However, analytical and experimental data are certainly insufficient to validate one mechanism over the other. It is known that quantum systems which are stochastic in the classical limit exhibit a considerable difference in behaviour when compared with the classical systems 18,19 . The basic distinction lies in the weak 20,21 stochastic properties of quantum systems. Strictly speaking, a correspondence in the behavior of a quantum system with that of a classical system can be expected only for times t < $t_{\rm d}$ where $t_{\rm d}$ is the time for the spreading of the wave packet. But this time is exponentially

small for stochastic motion. Nevertheless, it turns out that the main stochastic properties (such as diffusion) can take place on time scales with $t_d << t \le t_r$. Therefore it is of interest to determine to what extent the effects discovered in refs. [18-21] are significant in real systems, for instance, in the hydrogen atom in a time-dependent field.

In the present paper we have performed extensive quantum mechanical numerical studies of the hydrogen atom in a periodic delta function field (see also [22]). In other studies we have that some of the specific features of the behavior of this quantum system are typical of any periodic time-dependent external field. It also appears that by modulating the amplitude of S-function field it is possible to simulate a monochromatic perturbation.

II. RESPONSE OF A QUANTUM SYSTEM TO AN EXTERNAL TIME-DEPENDENT PERIODIC ELECTRIC FIELD

A quantum system under the influence of an external periodic time-dependent field of period T, can be characterized by the hamiltonian:

where H_O is the hamiltonian of the unperturbed system and H_{ext}(t) is the time-dependent hamiltonian corresponding to the external field. We assume that the external electric field is described by a superposition of periodic delta-functions of a specified period T. Thus,

$$H_{ext}(t) = eF_o \hat{\theta} \sum_{s} \delta(t-sT)$$
 (2.2)

where \hat{y} is a one particle operator, F_0 the strength of the field, and e the electric charge.

The form of the external field eq. (2.2) implies that the system is delivered a series of impulses at specified instants of time. Thus, before and after an impulse the propagation in time of the system is governed by the unperturbed hamiltonian H_0 ; each impulse, however, causing a modification in the amplitudes of the various states of the system.

A few comments about the form of the external field are in order.

- i) The fourier transform of the delta function field corresponds to the presence of all frequencies, of equal amplitude, in the external field. Thus, every time the system is imparted an impulse, there is sufficient scope for a large number of transitions and thus for the initial probability to disperse over a number of states.
- ii) In situations where the transition time (time taken by a system to make a transition from state n to n') is larger than the period T of the external field, then, the system can experience the effect of a train of delta function impulses during the transition. In such a case, the fourier decomposition of the external field (super position of periodic δ - functions) has features similar to the n-slit diffraction pattern. For large number of impulses, this pattern has a maxima when $\omega T = 2\ell G$ where ℓ is an integer. Thus a resonance can occur when the frequency wo of the external field equals the transition frequency; while the presence of higher harmonics can couple the system directly to the continuum and cause the damping of the resonance.
- iii) It is also important to realize that the time average of the chosen external field over one period is not zero, as in the case of a sinusoidal field. It is however, possible to generalize the definition of the chosen external field by considering a superposition of a train of delta functions acting alternately in opposite directions:

$$H_{ext} = H_{ext} + H_{ext}$$
, (2.3a)

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$$H_{\text{ext}}^{(1)} = e F_0 \hat{\partial} \sum_{s} \delta(t - 2sT),$$
 (2.3b)

and
$$H_{\text{ext}}^{(a)} = -eF_{o}\hat{V}\sum_{s} \delta(t-(2s+1)T)$$
. (2.3c)

Such a field has a zero time average over period 2T.

The dynamics of a quantal system described by the external hamiltonian eq. (2.2) is governed by the time-dependent Schrödinger equation.

$$i \pm \frac{\partial}{\partial t} \Psi(\vec{r},t) = H(t) \Psi(\vec{r},t)$$
 (2.4)

where $\Psi(\vec{r},t)$ is the corresponding time-dependent wave function of the system. The exact solution of this equation can be expressed in the form:

$$\Psi(\vec{r},t) = U(t,t_0)\Psi(\vec{r},t_0)$$
 (2.5)

where U(t,to) is a unitary time-evolution operator, given by:

$$U(t,t_0) = e^{-\frac{i}{\hbar}H_0(t-t_0)} - \frac{i}{\hbar}eF_0\hat{v}$$
(2.6)

Thus.

$$\Psi(\vec{r},t) = e^{-\frac{i}{\hbar}H_{o}(t-t_{o})} e^{-\frac{i}{\hbar}eF_{o}\hat{\vartheta}} \Psi(\vec{r},t_{o})$$
(2.7)

Since, the external field is periodic in time, eq. (2.7) exhibits quasiperiodic behavior, in which case:

$$\Psi(\vec{r},t) = \chi(\vec{r},t) e^{-\frac{i}{\hbar}(E_0 + \Delta E)t}, \qquad (2.8)$$

where, in accordance with Floquet theorem, the functions are periodic, satisfying the condition:

$$\chi(\vec{r},t) = \chi(\vec{r},t+T)$$
,

and E_0 is the unperturbed energy of the system and ΔE is the mean energy level shift, in general complex, caused by the external field. For each solution of eq. (2.8), there exists a value for the quasi-energy, $\Lambda = E_0 + \Delta E$ (defined modulo 2x $\frac{1}{2}$) for which the associated function $\chi(r,t)$ is regarded as the corresponding eigen-function [23-24]. It may be remarked that periodically driven systems, considered here, are distinct from the energy-conserving system. It is known, that for quantum systems, where the motion is bounded, the solutions of the time-independent Schrödinger equation, always yield a discrete

energy spectrum. As a consequence, the time evolution of both the wave function and its density matrix (or in the classical limit, the associated Wigner function) is nearly periodic. In classical mechanics this type of motion implies that the system is completely integrable. While for quantum systems, the near periodicity in motion suggests that asymptotically in time (t > \infty), the quantum system may never attain the character of a stochastic motion. Nevertheless, in such a long-time, the quantum motion can be ergodic. In contrast, for the non-conserving systems (like the one under study), the spectrum of quasi-energy in principle, be continuous. Therefore, for such systems one may expect a close resemblance to the stochastic properties of the corresponding classical systems.

III. HYDROGEN ATOM IN AN EXTERNAL IMPULSIVE FIELD

We consider hydrogen atom subjected to an external periodic impulsive uniform electric field (of the form of eq. (2.2) with $\vartheta = \hat{z}$) directed along the z-axis. This problem is exactly solvable, since the matrix elements of the field operator $\exp(-\frac{i}{\hbar} eF_0 \hat{z})$ (see eq. (2.7)) can be expressed in an analytical form provided the hydrogenic wave function are expanded in parabolic coordinates.

Since the hydrogen atom is a single electron system, the solution of the corresponding time-dependent Schrödinger equation exactly describes the time evolution of a (coherent) state

$$|z\rangle = e \qquad |n\rangle, \tag{3.1}$$

where

$$|n\rangle = Q_n^+ |0\rangle, \qquad (3.2)$$

describes the initial state of the electron, and $|0\rangle$ is the fermion vacuum, with a⁺(a) as the creation (annihilation) fermion operators. Eq. (3.1) can be expanded over a complete set of orthonormal basis states:

$$|z\rangle = B_{nn}|n\rangle + \sum_{m \neq n} B_{mn}|m\rangle,$$

= $B_{nn}[1 + \sum_{m \neq n} D_{mn} \alpha_{m}^{+} \alpha_{n}]|0\rangle,$ (3.3)

where B and D are some complex parameters, defined as:

$$B_{mn} = \langle m | e^{\frac{1}{\hbar}eF_0 \hat{Z}} | n \rangle,$$

$$D_{mn} = B_{mn} / B_{nn}$$
(3.4)

Thus the state |z> spans an infinite dimensional Hilbert space containing both discrete and continuum states of the Hydrogen atom. As a consequence, the state |z> acquires in time, both the spreading width as well as the escape width. Such a calculation thus goes beyond the usual studies of time-depen-

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dent quantal systems.

The hamiltonian for the Hydrogen atom in a periodic impulsive electric field can be explicitly written as (in what follows, we use Coulomb units, wherein $e = h = m_e = 1$):

$$H(t) = -\frac{1}{2} \vec{\nabla}^2 - \frac{1}{r} + \vec{F}_0 \hat{z} \sum_{s} \delta(t - sT),$$
 (3.5)

where

$$H_{o} = -\frac{1}{2} \vec{\nabla}^{2} - \frac{1}{r} , \qquad (3.6)$$

represents the hamiltonian for the unperturbed Hydrogen atom, $F_{\rm o}$ and T are respectively the strength (momentum) and the period (in atomic units, $t_{\rm o}$) of the external field.

The general solution of such a system is given according to eq. (2.7)

$$\Psi(\vec{r},t) = e \quad e \quad \Psi(\vec{r},0).$$
 (3.7)

Let us denote the initial state of the system at time t = 0 by a column matrix C:

$$\Psi(\vec{r},0) \Rightarrow \begin{pmatrix} c_1^{\circ} \\ c_2^{\circ} \\ \vdots \\ c_n^{\circ} \end{pmatrix}, \qquad (3.8)$$

where the component c_i^0 is the amplitude of the i-th discrete state of the hydrogen atom, satisfying the normalization condition:

$$\sum_{n=1}^{N} |C_{n}^{\circ}|^{2} = 1. \tag{3.9}$$

It is implicit from eqs. (3.8) and (3.9) that we consider only a subset of the spectrum of hydrogen atom; limiting ourselves to a finite number N (though, reasonably large) of discrete states.

From eqs. (3.5) and (3.7), the wave function between two consecutive impulses is governed by the unperturbed hamiltoni-

an Ho. The external impulses cause a mixing among the discrete states and with the continuum. Although, unbound states are not explicitly included in the calculations probability of ionization Pion, is defined as:

$$P_{ion}(t) = 1 - P_{s}(t),$$
 (3.10a)

where

$$P_{\Sigma}(t) = \sum_{n=1}^{N} P_{n}(t) = \sum_{n=1}^{N} |C_{n}(t)|^{2},$$
 (3.10b)

is the total probability in the discrete part of the spectrum. In eq. (3.10b), the amplitudes $c_n(t)$ evolve in time from the initial state (see eqs. (3.7) and (3.8)), due to the external impulse. Thus, in our calculations, the decrease in the probability among the discrete states is caused by coupling to the continuum. Since in our calculations, the process of recombination (i.e., the feeding back of the discrete states by the continuum) is ignored, P_{ion} corresponds to an instantaneous absorption of the ionized electron.

The truncation in the number of basis states is essential for computational tractability. In our numerical experiments, we have chosen a reasonably large number of basis states and in certain cases verified that by enlarging the basis space, the results do not change appreciably. Thus, the solution (eq. (3.5)) reduces to the calculations of $c_n(t)$, with n < N. From eq. (3.7),

$$C_n(t_{s+1}) = \sum_{m=1}^{N} V_{mn} C_m(t_s),$$
 (3.11)

where $c_n(t_{s+1})$ is the amplitude of the n^{th} state at the instant, $t_{s+1} = (s+1)T$, corresponding to $(s+1)^{th}$ impulse of period T; and $c_m(t_s)$ is the amplitude of the m^{th} state after the s^{th} impulse $(t_s = sT)$. The matrix, V, with elements V_{mn} is a product of two matrices; R, which describes the changes in the energy spectrum of the unperturbed states caused by the impulse

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$$\mathbb{R} = \begin{pmatrix} e & -i\lambda_{z}T \\ e & e \\ & & \\ & & \cdot & \\ & & \cdot & \\ & & & \\ & & \cdot & \\ & & & \\$$

and the matrix W, which describes the transitions between unperturbed states under the influence of a particular impulse,

$$W = \begin{pmatrix} W_{11} & W_{12} & \cdots & W_{1N} \\ W_{21} & W_{22} & \cdots & W_{2N} \\ \vdots & & \vdots & & \vdots \\ W_{NL} & W_{N2} & \cdots & W_{NN} \end{pmatrix}$$
(3.13)

Here, λ_n are the unperturbed eigenvalues of the n-th hydrogenic state and W_{ij} are the matrix elements of the external field;

 $W_{ij} = \langle U_i | e^{-iF_0 \hat{z}} | U_j \rangle$ (3.14)

where $u_i(\vec{r})$ and $u_j(\vec{r})$ are the unperturbed eigenfunctions of the hydrogen atom. Choosing the initial state $c_n(0)$ and calculating $c_n(t_s)$ dynamics of the system is completely specified.

IV. MATRIX ELEMENTS OF THE EXTERNAL FIELD

We consider hydrogen atom initially in a state with principal quantum number n > 1. Therefore, we assume that the hydrogen atom is axially symmetric about the z-axis along which the external field is directed. Thus, the projection $m = \langle \ell_z \rangle$ of the angular momentum along this axis is conserved. As a consequence, the wave functions can be labelled by the m quantum number. It is also convenient to use parabolic coordinates (ξ, h, ϕ) , defined in terms of the cartesian by the relations:

$$x = \sqrt{\xi} \frac{1}{\xi} \operatorname{Cos} \phi$$

$$y = \sqrt{\xi} \frac{1}{\xi} \operatorname{Sin} \phi$$

$$z = \frac{1}{2} (\xi - \frac{1}{\xi})$$

$$(0 \le \xi \le \infty, 0 \le \xi \le \infty, 0 \le \phi \le 2\pi)$$

$$(4.1)$$

Note that in these coordinates,

$$r^{2} = \frac{1}{4} \left(\xi + \xi \right)^{2}, \tag{4.2}$$

and the volume element dv is equal to

$$dv = dx dy dz = \frac{1}{4} (\xi + \xi) d\xi d\xi d\phi \qquad (4.3)$$

The corresponding unperturbed normalized wave functions for the hydrogen atom are given by [25]:

$$U_{n_{1},n_{2},m}(\xi,\xi,\phi) = \frac{2}{\sqrt{2\pi(na)^{3}}} \left[\frac{n_{1}! n_{2}!}{2n(n_{1}+|m|)!(n_{2}+|m|)!} \right]^{\frac{1}{2}} e^{im\phi}$$

$$\times \left[\frac{\xi \xi}{h^{2}a^{2}} \right]^{\frac{|m|}{2}} \frac{(\xi+\xi)/2na}{e} \left[\frac{|m|}{na} \left(\frac{\xi}{na} \right) \right]^{\frac{|m|}{2}} \frac{(\xi+\xi)}{na},$$

where

$$n = n_1 + n_2 + m + 1$$
, (4.5)

is the total principal quantum number, and n_1 and n_2 are the parabolic quantum numbers. In eq. (4.4), $L_q^{m_1}$ are generalized Laguerre polynomials which are normalized according to the convention of Gradshtayn and Ryzhik [26].

In the chosen basis, the matrix elements (eq. (3.14)) are characterized by five quantum numbers: (n_1, n_2, n_2, n_2, m) , and can be written in the form

Whining
$$= \langle U_{n_1 n_2 m} | e \rangle \langle U_{n'_1 n'_2 m} \rangle$$

$$(4.6)$$

Using eq. (4.4) we obtain,

$$W_{n_{1}n_{2}n'_{1}n'_{2}m} = \left(\lambda_{n}\lambda_{n'}\right) \frac{\alpha}{2} \left[\frac{n_{1}! n_{2}! n_{2}! n_{1}! n_{2}!}{(n_{1}+|m|)!(n_{2}+|m|)!(n_{2}+|m|)!(n_{2}+|m|)!} \right]^{\frac{1}{2}}$$

$$\times \int_{0}^{\infty} \int_{0}^{\infty} \int_{0}^{\infty} (\xi) g_{o}(\xi) (\xi + \xi) d\xi d\xi, \qquad (4.7)$$

where we have introduced

$$f_{o}(\xi) = \xi^{|m|} e^{-\beta_{nn'}\xi} \bigsqcup_{n_{1}}^{|m|} (\lambda_{n}\xi) \bigsqcup_{n'_{2}}^{|m|} (\lambda_{n'}\xi),$$

$$g_{o}(\xi) = \xi^{|m|} e^{-\beta_{nn'}\xi} \bigsqcup_{n_{2}}^{|m|} (\lambda_{n}\xi) \bigsqcup_{n'_{2}}^{|m|} (\lambda_{n'}\xi)$$
(4.8)

with the parameters:

$$\delta_{nn'} = \frac{iF_0 + \lambda_n + \lambda_{n'}}{2},$$

$$\lambda_n = \frac{1}{n\alpha},$$

$$\lambda_{n'} = \frac{1}{n'\alpha}$$
(4.9)

In the above expressions, a is the Bohr radius, equal to unity in the chosen units. The evaluation of the matrix elements $w_{n_1 n_2 n_1 n_2 m}$ depends upon two types of integrals of the form:

$$\int_{0}^{\infty} f_{o}(\xi) d\xi$$
 and $\int_{0}^{\infty} \xi f_{o}(\xi) d\xi$ (4.10)

By use of the recursion relation,

$$(\lambda_{n'}\xi) \bigsqcup_{n'_{i}}^{lml} (\lambda_{n'}\xi) = (2n'_{i} + |m| + 1) \bigsqcup_{n'_{i} - 1}^{lml} (\lambda_{n'}\xi) - (n'_{i} + |m|) \bigsqcup_{n'_{i}}^{lml} (\lambda_{n'}\xi) - (n'_{i} + 1) \bigsqcup_{n'_{i} + 1}^{lml} (\lambda_{n'}\xi)$$

$$(4.11)$$

it can be shown that all the integrals in eq. (4.7) reduce to the form

$$\frac{\int_{0}^{\infty} d\xi \cdot \xi^{|m|} e^{-b_{mn'}\xi} \prod_{n_{1}}^{|m|} (d_{n}\xi) \prod_{q}^{|m|} (d_{n'}\xi) = \frac{\Gamma(n_{1}+q+|m|+1)}{n_{1}!} \left(\frac{b_{mn'}-d_{n}}{b_{nn'}}\right)^{n_{1}} \left(\frac{b_{mn'}-d_{n'}}{b_{nn'}}\right)^{q} \\
\times \frac{1}{(b_{nn'})^{|m|+1}} \cdot \left[-(n_{1},-q;-n_{1}-q-|m|;\frac{b_{nn'}(b_{nn'}-d_{n}-d_{n'})}{(b_{nn'}-d_{n})(b_{nn'}-d_{n'})}\right), \tag{4.12}$$

where q is equal to n_1 or to n_1^{-1} , and F is a hypergeometric series. For convenience of further calculations, we make use of the transformation (see Appendix):

$$= \frac{(n_1+|m|)!(q+|m|)!}{|m|!(n_1+q+|m|)!} F(-n_1,-q;|m|+1;1-2)$$
(4.13)

Then the relation (4.12) becomes:

$$\int_{0}^{\infty} e^{-\delta_{nn'}\xi} \int_{m_{1}}^{|m|} (\lambda_{n}\xi) \int_{q}^{|m|} (\lambda_{n'}\xi) d\xi = \frac{1}{|m|!} \frac{(n_{1}+|m|)! (q+|m|)!}{n_{1}! q!} \left(\frac{\delta_{nn'}-\lambda_{n'}}{\delta_{nn'}}\right)^{n'} \left(\frac{\delta_{nn'}-\lambda_{n'}}{\delta_{nn'}}\right)^{q} \times \frac{1}{(\delta_{nn'})^{|m|+1}} \left[\left(-n_{1},-q;|m|+1;\frac{\lambda_{n}\lambda_{n'}}{\delta_{nn'}-\lambda_{n}}\right)^{n'} \left(\frac{\delta_{nn'}-\lambda_{n'}}{\delta_{nn'}-\lambda_{n'}}\right)^{q} \right]$$

$$\begin{split} & \bigvee_{n_{1}n_{2}n_{1}'n_{2}'m} = \frac{1}{(|m|!)^{2}} \bigvee \left\{ \frac{(n_{1}+|m|)!(n_{2}+|m|)!(n_{1}'+|m|)!(n_{2}'+|m|)!}{n_{1}! n_{2}! n_{1}! n_{2}!} \right\} \times \\ & \times \frac{(\lambda_{n}\lambda_{n}')^{|m|+2}}{2\lambda_{n}'} \cdot \frac{1}{|6|^{2(|m|+1)}} \cdot \left(\frac{\lambda_{n}}{6}\right)^{n_{1}} \left(\frac{\lambda_{n}'}{6}\right)^{n_{1}'} \left(\frac{\lambda_{n}}{6^{*}}\right)^{n_{2}'} \left(\frac{\lambda_{n}'}{6^{*}}\right)^{(4 \cdot 15)} \\ & \times d_{1}^{n_{1}} d_{2}^{n_{1}} d_{1}^{*} n_{2}^{*} d_{2}^{*} \left\{ G_{1} F(-n_{2}, -n_{2}'; |m|+1; d_{0}) + G_{2} F(-n_{1}, -n_{1}'; |m|+1; d_{0}) \right\}, \end{split}$$

$$G_{1} = (2n_{1}^{i} + |m| + 1)F(-n_{1}, -n_{1}^{i}; |m| + 1; d_{0}) - n_{1}^{i} \left(\frac{6}{6 - d_{n}^{i}}\right)F(-n_{1}, -n_{1}^{i} + 1; |m| + 1; d_{0})$$

$$-(n_{1}^{i} + |m| + 1)\left(\frac{6 - d_{n}^{i}}{6}\right)F(-n_{1}, -n_{1}^{i} - 1; |m| + 1; d_{0}),$$

$$G_{2} = (2n_{2}^{i} + |m| + 1)F(-n_{2}, -n_{2}^{i}; |m| + 1; d_{0}) - n_{2}^{i} \left(\frac{6^{*}}{6^{*} - d_{n}^{i}}\right)F(-n_{2}, -n_{2}^{i} + 1; |m| + 1; d_{0})$$

$$-(n_{1}^{i} + |m| + 1)\left(\frac{6^{*} - d_{n}^{i}}{6^{*} - d_{n}^{i}}\right)F(-n_{2}^{i} - n_{2}^{i} + 1; |m| + 1; d_{0}^{i}\right)$$

$$-(n_{1}^{i} + |m| + 1)\left(\frac{6^{*} - d_{n}^{i}}{6^{*} - d_{n}^{i}}\right)F(-n_{2}^{i} - n_{2}^{i} + 1; |m| + 1; d_{0}^{i}\right)$$

$$d_{1} = \frac{-(n_{2}^{1} + |m| + 1)(\frac{6^{*} - 2n^{1}}{6^{*}}) F(-n_{2}, -n_{2}^{1} - 1; |m| + 1; d_{0}), }{d_{2} = \frac{6 - 2n^{1}}{2n^{1}}; b = b_{nn'}; d_{0} = \frac{-1}{2n^{1}}.$$

It is clear from the above expressions that the calculation of the transformation matrix (eq. (3.11)) is not a simple problem even for one period. The matrix W is a $(N \times N)$ dimensional matrix, with each of its elements as an element of the four-dimensional matrix (recall that in our problem m = const).

The computational time for the calculation of the effects of one impulse grows as N^4 , where N is the number of unperturbed states of the hydrogen atom. However, the CPU time can be greatly reduced if the matrix elements are calculated once for all and stored in the fast memories of the computer. But, this is not always possible because of the limited size of the storage. For instance, for a computer with a storage M = 300,000 words, $N_{max} < M^{M} < 23$. In such cases, it is further useful to exploit the symmetries of the matrix elements. Nevertheless, for situations with N > 30 all the matrix elements have to be calculated each time, thereby increasing the CPU time.

In the present paper, we consider a particular case in which $m = \langle \ell_z \rangle = 0$. With such a choice, the expression for \mathbb{W} , is somewhat simplified. Separating the real and imaginary parts of $\mathbb{W}_{n_1 n_2 n_1 n_2}^{i_1 i_2}$ and making further transformations, one can represent $\mathbb{W}_{n_1 n_2 n_1 n_2}^{i_1 i_2}$ in a convenient form:

$$\begin{split} \mathcal{N}_{n_{1}n_{2}n'_{1}n'_{2}} &= Q_{n_{1}n'_{1}} e^{-i\Im(n'_{1}1)} e^{i\delta_{1}(n_{1}-n_{2}-n'_{1}-n'_{2})} e^{-i\Im(n'_{1}1)} e^{-i\Im(n'_{1}1)}$$

and the phases δ_1 and δ_2 are determined by the relations

$$tg\delta_1 = \frac{F_0}{d_{n'}-d_n}$$
; $tg\delta_2 = \frac{-F_0}{d_{n'}+d_n}$; $d_n = \frac{1}{n}$; $d_{n'} = \frac{1}{n'}$. (4.19)

There is no difficulty in deriving from the general expression (eq. (4.17)) the matrix element in a dipole approximation. In this case, the field needs to be weak:

$$F_{o} \ll \frac{|n\pm n'|}{nn'}$$
; $n \neq n'$. (4.20)

The dominant transitions occur between levels whose principal quantum numbers differ by unity $(n \rightarrow n' = n \stackrel{!}{-} 1)$. It follows then, that for the validity of dipole approximation

$$F_0 n^2 \ll 1$$
 (4.21)

For such a case, the first term in the expansion of $W_{n_1}^{n_2}^{n_1}^{n_2}$ in powers of F_0 exactly coincides with the known expression e^{27} and it is easy to obtain, if necessary, the next term in the expansion over the field F_0 .

V. NUMERICAL SIMULATIONS

We have performed extensive studies of hydrogen atom in highly excited states and for a variety of field-atom interactions. For calculations in which $n_0 \leq 9$, we have chosen $N_{max} = 20$, where N_{max} is the maximum number of discrete hydrogenic states included in the basic space. We have checked that by enlarging the basis space, the results do not change appreciably. In a similar fashion, for the cases in which the hydrogen atom is initially chosen to be in a state with $n_0 = 15$ or 17, we have consider $N_{max} = 30$. The dynamics of the system in each case has been followed through 300 impulses.

As already mentioned in Sec. II, the fourier spectrum of the external field:

$$F_o \delta(t-sT) \Rightarrow \frac{F_o}{T} \left(1+2\sum_{p=1}^{\infty} Cos \omega_p t\right)$$
 (5.1)

has frequencies, $\omega_p(=p\,\omega_o)$ that are multiples of the main frequency, $\omega_o=1$ It follows from eq. (5.1) that for a large

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number of impulses t(= sT, s >> 1), the zeroeth (or primary) harmonic corresponds to a constant electric field:

$$\xi_{o} = \frac{F_{o}}{T} \tag{5.2}$$

For convenience of comparison between the system under consideration and the system in which hydrogen atom is acted upon by a linearly-polarized monochromatic field, we introduce: a parameter ϵ , which is the amplitude of the periodic component of the impulsive field, eq. (5.1):

$$\mathcal{E} = \frac{2F_0}{T} \tag{5.3}$$

and a dimensionless perturbation parameter ξ , which is the ratio of the external field to the Coulomb atomic field ($\propto n_0^{-4}$) for a particular level n_0 of the hydrogen atom:

$$\xi = \varepsilon n_o^4 = \frac{2F_o}{T} n_o^4 . \tag{5.4}$$

Then the condition for smallness of the external field (weak field) can be expressed in the form:

where $\xi_{\rm cr}$ characterizes the onset of (significant) ionization. For example, $\xi = \xi_{\rm cr} = 1$, corresponds to the situation in which the atom can be instantly and completely ionized in one impulse. The parameters ξ and ξ serve as useful measures in studying the n_0 , F_0 and T dependences of the multiphoton absorption and ionization of the hydrogen atom.

a) RABI OSCILLATIONS

For field-atom interactions with $\xi < \xi_{\rm cr}$ one expects the validity of dipole approximation and hence a dominant $\Delta M = \frac{1}{2}$ transition. Depending upon the field parameters, $F_{\rm o}$ and T, the repeated application of the impulsive field of all frequencies can result in successive $|\Delta M| = 1$ transitions, thereby causing a diffusive growth of probability over the hydrogenic basis states. However, because of the inherent nonlinear dependence of the solution eq. (2.7) on $F_{\rm o}$ and T, the behavior of the system is not intuitively obvious. In fact computations reveal

some very striking peculiarities in the behavior of the system even for fairly weak fields.

Figure 1 exhibits some of the features of the hydrogen atom subjected to weak perturbations. Plotted as a function of time (or the number of impulses) is the probability $|c_n(t)|^2$ among the discrete states of the hydrogen atom. At time t = 0, the atom is assumed to be in the state with $n = n_0 = 7$. The external field is characterized by $F_0 = 0.0015 \text{ volt-cm}^{-1}$ -sec and T = 2627t_o, where the atomic unit of time, $t_o = 2.42 \times 10^{17}$ sec. Thus, the external field corresponds to ξ = .0027 a.u. From fig. 1, there is dramatic localization of the probability about the initial state, although at the end of 300 impulses, the atom is about 15 percent ionized. It is remarkable that there is no evidence of diffusive growth of probability over the discrete state. Instead, after a few impulses, the initial state with n = 7 is seen to couple at the most to the state with n = 8, while the ionization is caused by the direct coupling to continuum. That for certain values of period T, the initial state is strongly coupled to one other state whose principal quantum number n differs by unity from that of the initial state, appears to be a general pattern in all the calculations. In all such cases, the total probability in the space of discrete states is almost entirely exhausted by this pair. Such a case is illustrated by fig. 2, which shows the time dependence of the probability P_n for two states with $|n\rangle = n_0 =$ = 9 and n = 10 . At time, t = 0, the hydrogen atom is assumed to be in the state with parabolic quantum numbers with $n_1 = n_2 = 4$, m = 0; corresponding to principal quantum number $n = n_0 = n_1 + n_2 + m + 1 = 9$. The period T of the external field is chosen to correspond to the transition from the state with $|n = 9\rangle$ to the state with $|n = 10\rangle$.

Thus:

where

$$\omega_0 = \Omega = \frac{1}{2} \left[\frac{1}{n_0^2} - \frac{1}{(n_0 + 1)^2} \right]. \tag{5.6}$$

The perturbation parameter & has the values:

$$\xi = \epsilon n_0^4 = \begin{cases} 0.005 \text{ a.u. for } n_0 = 9 \\ 0.0075 \text{ a.u. for } n_0 = 10 \end{cases}$$
 (5.7)

corresponding to the situation in which the probability $|c_n(t)|^2$ goes over, in time, from the state with $|n_0| = 9$ to the state with $|n_0| = 10$ and vice-versa. In the following, we consider $\xi = 0.005$ a.u. Figure 2 shows a quasi-periodic nature of the interaction between the two states with n = 9 and 10, and the external field. It turns out, however, that behavior is considerably more complicated than a simple two state resonance. There is damping which arises from the removal of probability by ionization and also a system of beats (case of Rabi oscillations). There occur significant differences between an ideal two state resonance and the one seen above. In that, the external field mixes the states with different parabolic quantum numbers (n_1, n_2) , which are not degenerate in energy. In fig. 2, the two states involved are explicitly:

 $|n_0=9\rangle = U_{440}(\xi,\xi),$ and $|n_0=10\rangle = \frac{1}{\sqrt{2}} \left[U_{450}(\xi,\xi) - U_{540}(\xi,\xi) \right].$ (5.8)

A feature of our model is that the external field contains arbitrarily high frequencies, as a consequence there is sufficient scope for direct ionization. It is mainly this direct coupling of the bound hydrogenic states to the continuum, that results in decreasing the total probability in the discrete basis space. For the case presented in fig. 2 the probability for ionization over 300 impulse is negligibly small ($P_{\rm ion} \approx 3\%$). A closer inspection of fig. 2 shows that the system recurs to almost the same state repeatedly often, in time, a feature similar to that observed in one-dimensional problems. Our earlier analysis of the behaviour of the system in a weak impulsive field shows that with decreasing $F_{\rm o}$, the behaviour of the system closely resembles an idealized two-level system. In particular, for very small $F_{\rm o}$ the period of oscillation is proportional to $F_{\rm o}$.

B. COHERENT OSCILLATIONS IN A STRONG FIELD

For intense external fields, the dipole approximation is inapplicable and the matrix elements of the interaction Wn,non,no become nonlinear in Fo. With increasing Fo direct ionization becomes more probable. This causes a considerable reduction in the total probability among the discrete levels of the H-atom. However, astriking feature evident from the calculations is that even in cases where Pion is large, strong correlations between the neighboring states persist for a long time. Again, only a few neighboring (resonant with the field) states are excited and no considerable diffusion is observed in the upward direction of the spectrum. A typical situation of this behavior occurs for \$ \approx 0.02-0.03 a.u. and for the initial state with $n_1 = n_2 = 4$, corresponding to $n_0 = 9$. Figure 3 presents three examples for different values of & and T. Figures 3(a), 3(b), 3(c)) illustrate the effect of keeping the field strength fixed (F = 8×10^{-3}) and changing the period T. For T = 5000 t₀ (fig. 3(b)) we are close to the $9 \leftrightarrow 10$ resonance (the exact resonance occurs at T $(9 \leftarrow 10) = 5357 t_0$) while T = 4000 t₀ (fig. 3(a)) produces a somewhat detuned 9 → 8 resonance, the natural period of which is 3832 to. From figs. 3(a) and (b), it is manifest that probability is again shared mostly by two states. The oscillations between the two states being strictly correlated with each other. Also, in time there is a decrease in amplitudes of these two states caused mainly by the direct coupling to the continuum. From fig. 3(c) increasing the period to 6000 to leads to the altogether more complicated behavior. Here states with n = 9, 10 and 11 all have appreciable probability. The principal feature again is a two--state resonance between states with n = 9 and 11. The natural period for this resonance is 3079 to and so presumably the transition occurs on the second harmonic of the external field. Neither the 9 ← 10 nor the 10 ← 11 resonances is conveniently close to T = 6000 t.

It should be pointed out that two-states resonances persist even in cases where the system shows strong damping due to direct ionization. Figures 2, 3(b) and 4 form a sequence in which T is close to the natural period in each case but F_o has

the values 2×10^{-3} , 8×10^{-3} , and 1.6×10^{-2} a.u. The change in the period of the oscillation with increasing F_0 is apparent. For very small values of F_0 , the period of the oscillation is proportional to F_0 . From fig. (4) the two-state resonance clearly persists up to 300 impulses with the loss of most of the probability by ionization. Even in such a strong field ($\xi = 0.04$ a.u.) we see no evidence of diffusion over discrete basis.

An interesting situation arises, for the case with T = = 400 t_0 , n_0 = 9 and F_0 = 0.008, corresponding to a very strong perturbation parameter \ = 0.26 a.u. From fig. 6, we notice that the ionization probability increases dramatically to about 30 per cent in first 40 impulses and thereafter a new regime arises, in which the time evolution of the system shows a near saturation in the Pion. Here again the probability among the bound states is mostly exhausted by states with $n_0 = 9$ and n = 10. Fig. 5 shows a time variation of the probability in these two states. It is seen that after an initial rise and fall respectively in the intensities of the states with n = 10and 9, the probabilities oscillate with a mean value of about 12 percent for the n = 10 state and about 35 percent for the n = 9 state. It may be remarked that the period $T = 400 t_0$ of the external field is far too small compared to the natural period of the 9-10 transition, which equals 5357 to. Thus the system experiences a coherent influence of a substantially large number of impulses (\approx 12) during its natural transition period. As a consequence, the main frequency $\omega_0 \simeq 0.0157 t_0^2$ of the external field couples the n = 9 state directly to the continuum; thereby causing a substantial drop in the probability of the n = 9 state during the early stages of the evolution. The coherent influence of the large number of impulses experienced by the system during its natural transition period, eventually forces the system to resonate with the external field. Thus, for later times, the observed near constancy of the probabilities in the n = 9 and 10 states is highly suggestive of "forced oscillations", in which the time-dependent phases of the states with n = 9 and 10 adjust to those of the external field. Thus, these two states constitute the near "eigen-states" of the total Hamiltonian.

According to the classical description, a system subjected to intense periodic perturbations should under certain conditions exhibit a stochastic behavior. The mechanism for the occurance of such a behavior depends on the interaction between the nonlinear resonances in systems subjected to periodic perturbations. The nonlinearity in the Hamiltonian is significant for the appearance of such resonances and leads to an unperturbed motion containing large number of harmonics which are multiples of the Keplerian frequency $\Omega \approx 1/n^3$. This implies that even in the case of a harmonic time dependence of the external field (monochromatic wave), the resonance relation:

 $\omega \approx k \Omega_{\kappa} = k n_{\kappa}^{-3}$, (k is an integer), (5.9)

can be fulfilled for different unperturbed levels nk. For an isolated nonlinear resonance (i.e. when the influence of all other resonances is neglected), the oscillations of the action variable are limited. This results only in a regular exchange between the group of levels captured by the resonance. With increasing field strength, the width of the nonlinear resonance (in frequency and, hence in action) grows, and can become comparable to the distance between the neighboring resonances. In such a case, stochastic diffusion over the overlapped resonances occurs. Quantum systems subjected to periodic impulses when compared to their corresponding classical analogs based on the concepts of stochastic diffusion indicate that, for "quantum stochastic diffusion" to occur every non-linear resonance must capture a large number of levels of the unperturbed system [28]. Our numerical experiments with the H-atom demonstrate that an intense exchange between the neighbouring levels arises for large Fo. This exchange gives rise to the spreading of the probability initially concentrated in one level. Fig. 7a illustrates the probability distribution over 30 hydrogenic levels, for different times t. Initially hydrogen atom is assumed to be in the $|n_0 = 9\rangle$ state. The perturbation parameter, $\xi = n_0^4 \simeq 0.052$ a.u. From figure 7 such a perturbation leads simultaneously both to the diffusion over discrete

levels and direct ionization. Since for a constant F_0 , direct ionization increases with increasing n_0 , the sharp decrease in the initial probability is mainly due to diffusion over the states with $n > n_0$, from each of which, in turn, direct ionization occurs.

The situation indicated in figure 7 is typical for large values of $\gtrsim 0.05$ a.u. Because of strong direct ionization, observation in time of the diffusion over the discrete basis becomes difficult. Figure 8 shows the probability of direct ionization on the parameter \lesssim (and/or F_0) at the end of s-number of impulses. Note a sharp increase in the ionization, for values of $F_0 > 0.14$. The latter saturation is most likely due to the onset of coherent (forced) oscillations, described in Sec. V.B.

It is worth emphasizing that ionization is, in essence, connected with the probability diffusion upward the spectrum and is enhanced when higher levels, $n\gg n_o$ are excited. However in situations where the ionization on the main frequency ω_o is possible, there exists a limiting value of $n=n_\omega$, above which (for $n>n_\omega$) the probability among the discrete states does not grow. If the frequency of the external field is chosen to correspond to the resonance between the states $|n_o>$ and $|n_o+1>$, then the value of n_ω is given by

$$n_{\omega} = \frac{n_{o}(n_{o}+1)}{\sqrt{2n_{o}+1}} . (5.10)$$

Thus for $n_0 = 5,9,13,17$ (the initial states for which the numerical experiments have been performed), we have

$$n_0 = 5$$
 9 13 17 (5.11) $n_{\omega} = 9$ 21 35 52

This suggests that for $n_0 = 5$ and 9 the basis space spanned by levels with n < N = 20 should suffice for the calculations. Indeed, calculations with an increased basis space, with N = 30 showed no noticeable difference in the dynamics of the system.

Among the other effects of importance to the problem under study is the decrease of the ionization threshold caused

by the constant electric field due to the presence of zero harmonic, $\xi_0 = F_0/T$, of the external perturbation. A rough estimate for the critical field ξ_c is given by [27]:

$$\mathcal{E}_{c} \approx \frac{1}{16n^{4}} . \tag{5.12}$$

However, if one takes into account the shift of the Stark levels, (see, e.g., Ref. [29]), then the minimum value of \mathcal{E}_c is obtained for the cases with $n_1 = n-1$ and $n_2 = 0$. Thus,

$$\varepsilon_{\rm c} \sim 0.13 \, {\rm n}^{-4}$$
 (5.13)

Using eq. (5.13) we obtain an estimate for the threshold value for n_a :

$$n_s \sim n_o \left[2 \frac{0.13}{\xi} \right]^{1/4}$$
 (5.14)

For a fairly strong perturbation $\xi \approx 0.04$ a.u., we have

$$n_o \approx 1.7 n_o$$
 (5.15)

which for n_0 = 5, 9, 13, and 17 gives respectively n_g = 9, 15, 22 and 29. For small n_0 the diffusion can occur only over a small number of levels $n < n_g$ (see also Fig. 7). Thus it follows, that for a reliable observation of the stochastic diffusion in time, n_0 needs to be sufficiently large and the total number N of the levels under consideration should not be less than N ~ $2n_0$.

The problem can however be simplified by studying the conditions under which the system exhibits a characteristic feature of diffusion in the initial stages, followed by an intense exchange between unperturbed levels. Figs. 3 and 4 depict a typical behavior of such a phenomenon. There is a short characteristic time for the spreading of probability from an initial state $|n_0\rangle$ to the other neighbouring states. Beyond this, the probability in the state $|n_0\rangle$ varies just about an average value, any further decrease occuring comparatively slowly.

As an example let us inspect fig. 4 rather closely. Fig. 9 shows a blown-up plot of fig. 4 but over a shorter period of time, t < 40 t_o. From fig. 9, curves 1 and 2, it is clear that the correlated oscillations of the probabilities in the states

with n_0 = 9 and n = 10 are set up after about three impulses. Also during this stage, the sum of the probabilities P_9 + P_{10} shows a sharp decrease, followed by its near constancy over a long period of time. The total probability (curve 5) is weakly decreasing indicative of a weak ionization. Let us now introduce a quantity β , as a measure of the correlation between the states n_0 and n_0 + 1 and defined by the ratio:

$$\beta = \frac{P_{n_0} + P_{n_0+1}}{P_{\Sigma}} \tag{5.16}$$

where $P_{\rm T}=1-P_{\rm ion}$ is the total probability over the bound hydrogenic states. Clearly, $\beta \sim 0.5$ defines a critical value, above which the motion is stable, and below which the motion may be regarded as 'stochastic'.

Fig. 9, curve 3 shows the time-variation of β . The values of β oscillate about a mean value (curve 4) of about 0.7, even for such a fairly strong perturbation considered here. Thus indicative of 'stable' motion of the system at least for some stages of the time-evolution.

Figs. 10 and 11 exhibit the variation in β and P_{Σ} with increasing ξ , for different choices of $|n_0\rangle$, with a uniform distribution over the parabolic quantum numbers, $n_1 = n_2$ (it corresponds to $\ell = 0$ [30]). Although, classical estimates do indicate the ℓ -dependence $(n_1 \neq n_2)$ of ξ_{cr} for the occurance of 'stochastic' behavior, for the present we consider the cases with & = 0. From figs. 10 and 11, the computations reveal that for {< 0.03 a.u., the motion is considerably more stable for the case with $n_0 = 9$ than for those with $n_0 = 13$ or 17. The dramatic decrease of $P_r \sim 0.3$ for $\xi \approx 0.05$, for $n_0 = 9$ arises mainly due to the direct ionization from the states, n_0 and n_0 + 1 and is more a consequence of increasing F_0 than ξ . For the cases, with $n_0 = 13$, and 17, the critical value of β (\sim 0.5) corresponds to a value, ξ = 0.03 - 0.04 a.u. For {< 0.03, a.u., the initial distribution stays highly localized with a weaker ionization. It is seen also that for no = 5 the ionization is very strong. The reason is a rather small threshold Nw (5.11). In addition, for this case, the multiphoton excitation proves to manifest itself much stronger

VI. ANALYTICAL ESTIMATES AND DISCUSSIONS

A. Stochastic Diffusion

As mentioned in Section I, for a highly-excited atom, besides tunnelling and multiphoton ionization stochastic diffusion can play a significant role in the ionization process. Such a diffusion is encountered for a wide class of classical non-linear systems, and is mainly featured by the absence of random forces in the system. The stochastic diffusion occurs in strictly deterministic systems; it can arise even in the systems with a few degrees of freedom. Under certain conditions for non-linear classical systems, a local instability of motion appears for which the otherwise closed trajectories in a phase space show rapid exponential divergence. Because of the limited phase volume, this results in a rapid mixing of the trajectories and, as a consequence in the irregularity (stochasticity) of motion of the system. In an autonomous system, the exchange of energy between different degrees of freedom is of random nature, while in the nonautonomous one, both the stochastic diffusion and the unlimited growth of energy in the system occur under the influence of the external force.

The criterion for the appearance of stochastic diffusion is based on the interaction between the numerous non-linear resonances excited in the system under the influence of a periodic perturbation. Let us consider the case of hydrogen atom, populated in a state with parabolic quantum numbers $n_1 = n_2$ ($\ell = 0$) and m = 0. Following ref. [2], the Hamiltonian of the corresponding system, regarded as classical, can be written as:

$$H = -\frac{1}{2n^2} + F_0 n^2 \delta(t - sT) \left\{ -\frac{3}{2} + 2 \sum_{k=1}^{\infty} z_k \cos k \lambda \right\}, \quad (6.1)$$

where n and λ are canonically conjugate defining the action and the phase. The electric field is assumed to be directed parallel to the electron orbit and the fourier component of the dipole moment of the electron [31] is given by:

$$n^2 2e_k = \frac{n^2}{k} \, J_k(k),$$
 (6.2)

and the orbital eccentricity, $e = \sqrt{1-\ell^2/n^2} = 1$. Expanding the delta function in fourier series, eq. (6.1) can be expressed as follows:

$$H = -\frac{1}{2n^2} - \frac{3}{2} \epsilon_0 n^2 + 2 \epsilon n^2 \sum_{k,p=1}^{\infty} Cosp \omega_0 t \cdot Cosk \lambda$$
 (6.3)

For the values of the field F_0 ($\xi_0 n^4 < 0.08$) considered so for, the second term in eq. (6.3) can be neglected in comparison with the first term, and the resonance relation then has a form

 $p\omega_o \approx k\lambda = k\Omega$, (6.4)

where 2 is the frequency associated with the Keplerian motion of the electron in its orbit. The value of Ω is energy-dependent and is given by $\Omega \approx 1/n^3$. Unlike the monochromatic external field for which p = 1, the perturbation in eq. (6.3) contains a large number of the resonant terms. As a result, the critical value of ξ_{cr} , at which the resonances overlap, is expected to be lower than in the case with a monochromatic perturbation. The strongest resonance occurs when p = k = 1 (the main resonance). Here the main frequency of the perturbation equals the keplerian frequency: $\omega_0 \approx \Omega \approx 1/n_0^3$. However, as seen from eq. (6.4), same resonance condition also holds for any p = k. This implies that in order to study the effects of the main resonance, contribution of all the terms with different p = k should be taken into account. If we neglect all the other resonances and define new canonical variables. I = = n - n and $\delta = \lambda - \omega_t$, we obtain the Hamiltonian for the resonance.

$$H_1 = -\frac{3I^2}{2n_0^4} + \epsilon n_0^4 \sum_{k=1}^{\infty} 2e_k \cos k \epsilon$$
 (6.5)

This Hamiltonian is independent of time and describes the oscillations of the action variable I in the vicinity of the resonance value $n_0 = \Omega^{-1/3}$. Using eq. (6.5), the maximum variation of the action is given by:

$$(\Delta I)_{\text{max}} = (\Delta n)_{\text{max}} = \pm 2 n_0^3 \left[\frac{\epsilon}{3} X_i \right]^{1/2},$$
 (6.6)

where, with the use of eq. (6.2),

$$\chi_{i} = \frac{1}{2} \sum_{k=1}^{\infty} x_{k} [1 - (-1)^{k}] = \frac{1}{2}$$
 (6.7)

and the Halfwidth of the resonance (in frequency) is given by

$$(\Delta \Omega)_{11} = \frac{d\Omega}{dn} (\Delta n)_{max} = \pm \frac{2}{n_0} \sqrt{3} \times \overline{X}_1. \qquad (6.8)$$

The expression eqs. (6.6-6.8) define the amplitude of the non-linear oscillations, in the energy and frequency domain, once the system is subjected to an external field whose frequency is equal to the Keplerian frequency of the electron. These expressions are applicable if i) the perturbation is weak (i.e. the situation in which all but one resonance may be ignored), and ii) ΔI is small as compared to n_0 . For a quantum system, described within the semi-classical approach (when $n \gg 1$), an additional condition must be satisfied, in that the number of quantum states involved in the non-linear resonance should be fairly large [28].

When the perturbation is increased, while still remaining within the regimes of the applicability of a perturbation theory (${\rm en}^4 < 1$), the usefulness of the existence of an isolated resonance breaks down. In such cases, the interaction between the neighbouring resonances becomes important, which gives rise to stochasticity. Thus the criterion for the occurance of stochasticity consists of finding the condition for which neighbouring non-linear resonances overlap. For this, it is then required to analyse the resonant structure of the perturbation and the identification of the most important resonances. A detailed analysis shows that for the case of hydrogen atom, when the frequency ω_0 of the external field is approximately equal to the Keplerian frequency $\Omega \sim 1/n_0^3$, the strongest resonance occurs when k = 3 and p = 2. According to eq. (6.4), it follows that for this resonance,

$$\Omega_{pk} = N_{pk}^{-3} = \frac{P}{k} \Omega_o = \frac{2}{3} \Omega_o, \qquad (6.9)$$

where nok determines the location of the resonance:

$$n_{pk} = n_o \left(\frac{k}{p}\right)^{1/3} = {3/2 \choose 2}^{1/2} n_o$$
 (6.10)

Introducing the new action-phase variables:

$$I_{pk} = n - n_{pk}$$
; $G_{pk} = k\lambda - p \omega_{ot}$, (6.11)

we obtain, similar to eq. (6.5),

$$H_{pk} = -\frac{3I_{pk}^{2}}{2n_{pk}^{4}} + En_{pk}^{2} \sum_{r=1}^{\infty} \chi_{3r} \cos(r \epsilon_{pk}). \tag{6.12}$$

For the coinciding resonances, $r(3\lambda - 2\omega_0 t) \sim 0$, while from eq. (6.12) the halfwidth of the resonance in frequency is

$$(\Delta \Omega)_{pk} = \frac{2}{n_{pk}} \left[3 \xi X_3 \right]^{1/2},$$
 (6.13)

where

$$\chi_3 = \frac{1}{2} \sum_{r=1}^{\infty} \mathcal{X}_{3r} \left[1 - (-1)^r \right] \approx 0.08$$
 (6.14)

Having obtained the total halfwidth $(\Delta\Omega)_{11}+(\Delta\Omega)_{31}$, and knowing Ω_{31} , between the two resonances, the condition for their overlap can be obtained. As shown in Ref. [13], the effective overlap, at which the trajectory goes randomly from one resonance to the other, is achieved whence

$$\mathcal{K} = 2.5 \, s^2 = \frac{\xi}{\xi_{cr}} > 1 \,\,, \tag{6.15}$$

where

$$S = \frac{(\Delta \Omega)_{11} + (\Delta \Omega)_{31}}{\Omega_{11} - \Omega_{31}}; \quad \Omega_{11} \equiv \Omega_{0}. \quad (6.16)$$

For the resonances under consideration, we eventually obtain

$$\xi_{cc} = \xi_{cc} n_o^4 \sim \frac{1}{220} . \qquad (6.17)$$

The analysis shows that for $\xi > \xi_{cr}$, two resonances with p = 2; k = 3 and p = 1; k = 2 overlap. It turns out that the critical value of perturbation for the overlap of the resonances with $n > n_2$ (k = 2, p = 1) decreases with increasing n. This suggests that the critical value of { for the onset of diffusion from no is determined by only a few low-order resonances. For a monochromatic perturbation (p = 1) it is sufficient to consider only two resonances with k = 1 and k = 2 (see Ref. [2]). However in the case of & -function external field the high-order resonances occur close to the main resonance (p >> 1; k > p) and thus can overlap under very small perturbation (in the limit, $\xi_{cr} \rightarrow 0$ when $p \rightarrow \infty$). For the purpose of the further comparison of the classical results with the quantum calculations, it seems sufficient to take into account only the two resonances mentioned above. A possible reason for this is that, for other resonances k is rather large (k>5) and the number of quantum levels involved in the resonance turn out to be ≤ 1, because of sharp decrease in the width of the resonance.

The estimate of ξ_{cr} eq. (6.17) differs from that for monochromatic perturbation (Ref. [2], for which

$$\xi_{cr} \sim \frac{1}{84}$$
 (6.18)

Thus for an impulsive periodic field, considered in the present paper, the values of critical fields are smaller by a factor of 2.6 compared to the monochromatic field strength.

The validity of the semi-classical approach is related to the capture of a large number of levels Δn by the non-linear resonance. An estimate for Δn can be obtained from eq. (6.6) according to which.

$$\Delta n = 2 (\Delta I)_{max} = 4 n_0 \frac{k}{p} \sqrt{\frac{3}{3}} X_k \sim 0.33 n_0 \frac{k}{p} X_k^{1/2}$$
 (6.19)

For the main resonance, p = k = 1, we obtain for various values of n_0 :

n _o	9	13	17
n	2.1	3.0	3.9 if (₹~0.22 a.u.)
n	3.0	4.2	5.6 if (\(\cap \cap 0.04 \) a.u)

It is clear that the condition

A = >> 1	11 001
Δn >> 1,	(6.20)

can play an important role in limiting the stochastic diffusion for even sufficiently large n_0 and ξ . Nevertheless, the numerical results show that even for $\xi=0.04$ a.u., and $n_0=13$ and 17 an intense exchange occurs only between a small number of states in the vicinity of n_0 . This is contrary to the classical estimates, according to which the resonance overlap condition becomes weaker with increasing n_0 . From eq. (6.19), for large k the number of levels An captured by the resonance grows as $k^{1/6}$ thereby satisfying the condition eq. (6.20). In contrast, the estimates (eq. (6.10) with p=1) for the resonant values of the action n_0 , corresponding to the location of the overlapping resonances of higher harmonics, are given as:

no	$n_2(k=2)$	n ₃ (k = 3)	$n_4(k = 4)$
9	11	13	14.3
13	16.4	18.7	20.7
17	21.4	24.5	27

B. Influence of a Constant Field Component

As mentioned in Section II the external δ -function field has a constant component ξ_o . In deriving the analytical estimates, the influence of ξ_o in eq. (6.3) has been neglected, although without any justification. Our analysis of the numerical results suggests that the decrease in the total probability \mathbf{p}_{Σ} , though caused primarily by direct ionization, is enhanced due to small ionization threshold which depends on

 ξ_0 . In order to further understand the effects of ξ_0 , we have also performed a series of numerical experiments.

In the first set of calculations, we have considered hydrogen atom subjected to perturbation eq. (2.3) but with the constant component of the electric field & set to zero. The amplitude of the first harmonic has been retained at its original value. Thus,

$$H_{ext} = \frac{F_o}{2} \geq \sum_s \delta(t - sT) - \frac{F_o}{2} \geq \sum_s \delta(t - sT - \frac{T}{2}), \qquad (6.21)$$

or

$$H_{ext} = \frac{2F_o}{T} \sum_{p=1}^{\infty} Cospw_ot, \quad p-odd.$$
 (6.22)

The behavior of the system presented in Fig. 4 for ($\mbox{$>$} \approx 0.04$, $n_0 = 9$), now proves to be considerably more stable. In that, the average value of $\mbox{$<$>$>$}$, which characterizes the relative intensity in the states $|n_0\rangle$ and $|n_0|+1\rangle$, increases from 0.70 to 0.84, whereas the probability for direct ionization decreases sharply ($P_{\Sigma} = 0.94$ instead of 0.79). The probability distribution over the hydrogenic basis is further localized; the effective excitation practically involves only two states: $|n_0\rangle$ and $|n_0|+1\rangle$. It should be mentioned however that the difference in the behaviour is not entirely due to the absence of the constant electric-field component, but also due to the absence of even harmonics, with $p=2,4,\ldots$

In another set of calculations, besides the perturbation V_1 eq. (2.2) of period T and amplitude F_0 , a similar perturbing field V_2 , but of period $T_1 = T/5$ and amplitude $F_1 = -F_0/5$ has been added. Thus, the perturbing hamiltonian is chosen to be of the form: $H_{\rm ext} = F_0 \sum \delta(t-sT) - \frac{F_0}{5} \sum \delta(t-s'T/5)$. For such an external field every fifth impulse from V_2 coincides with an impulse from V_3 . In contrast to the perturbation eq. (2.2), such a perturbation contains no Oth, 5th, 10th, etc. harmoniss. Numerical results obtained for the cases presented in fig. 4 show similarities in behavior. For $H_{\rm ext}$ given above, the average value $<\beta>\sim 0.76$ while total probability $P_5\sim 0.85$ (for $t_m=40$). This close agreement between the results obtained with and without the constant component in the perturbation

suggests that the constant field component ξ_0 is not important for the dynamics of the system.

C. Role of Initial Distributions

Analytical estimates [2] indicate that diffusion depends strongly on the orbital angular momentum quantum number ℓ . For & small, the magnitude of the critical perturbation parameter, &cr, appears to be minimum. With increasing &, &cr increases sharply. This can be appreciated from the fact that for small &, the orbits extend in the direction of the external electric field. It is thus natural that for such cases, the influence of the perturbation will be stronger than for the (near) circular ones. Using the transformations for the change of basis from spherical to parabolic coordinates, [30] we have studied several cases with the initial distributions over the parabolic quantum number (n, n) corresponding to $\ell = 0,1$ and $n_0 - 1$. The state with $\ell = 0$ corresponds to a uniform distribution, n₁ = n₂ for a fixed n₀. Numerical results for the case of a hydrogen atom, initially in the state no = 13, under the influence of a periodic delta function field characterized by $\xi = 0.04$ a.u., indicate that $\langle \beta \rangle$ remains nearly constant (~ 0.5), for $\ell = 0.1$ and $n_0 - 1$. However, in going from $\ell = 0$ and 1 to $\ell = n_0 - 1$, the distribution over the hydrogen levels becomes considerably sharper, with a weaker excitation of the higher levels. Correspondingly, the direct ionization decreases. Thus, for $\ell = 0$ and $\ell = 1$, the total probability P2 is equal to 0.72 (Fig. 11) and 0.64 respectively, while for $\ell = n_0 - 1$, P_{Σ} varies from 0.93 to 0.96).

Of special interest is the study involving parabolic states with a large ratio $n_2/n_1 \gg 1$. It turns out that this ratio remains approximately conserved in time, and the excitation covers only these specific states. Such a feature then allows us to employ the approximation of a onedimensional hamiltonian describing strongly extended orbits $\begin{bmatrix} 32-34 \end{bmatrix}$. Such a model is also used in the description of the behaviour of an electron above the surface of liquid helium in an external time-dependent field $\begin{bmatrix} 35-36 \end{bmatrix}$. Indeed, the numerical experiments with the parabolic initial distribution $(n_1 = 0, n_2 = 12)$ for $n_0 = 13$

and $\xi \approx 0.04$ and 0.02 show that the excitation covers, mainly, the states with $n_1 = 0$. However, for large ξ the states with $n_1 = 1$ begin to get excited. Further analysis of such model studies is in progress.

D. Multiphoton Excitation

Besides the stochastic diffusion, multiphoton excitation is regarded as a major mechanism for the ionization of atoms, when $\chi \gtrsim 7$. The relationship between these two mechanisms of ionization is intimately related to a more general question concerning the validity of semi-classical approximation for the description of quantum system with n >> 1. Comparison between the classical and quantum one-dimensional model calculations [32] show that even for very large n = 50 to 100, strong multiphoton resonances dominate over the stochastic diffusion, which substantially limits the use of a classical description.

In our calculations involving two degrees of freedom (n_1,n_2) , both multiphoton ionization and direct ionization are implicitly incorporated. Numerical experiments for various n_0 , and ℓ , suggest that for small perturbations multiphoton resonances play a significant role in the ionization process. However, with stronger perturbations their influence becomes weaker. Also, multiphoton processes become important when there is no mixing between n_1 and n_2 , i.e. when the situation is close to that of one-dimensional case. Such a conclusion is born out by the case with parabolic initial excitation $n_1 = 0, n_2 = n_0 - 1$. Although this question needs further study it is somewhat clear that the role of multiphoton resonances in a system with two degrees of freedom is considerably weaker than in the one-dimensional model.

E. Adiabatic Switching of the External Field

In order to compare the behavior of hydrogen atom under an impulsive (delta-function type) external field, with that of the system under an external perturbing field that grows slowly in time, we have performed an additional numerical study of hydrogen atom with a perturbation that increases slowly in time. As in ref. [15], the amplitude dependence of such a perturbing field F(t) was chosen to be of the form:

$$F(t) = \begin{cases} F_0 \exp(\chi(t-t_0^*)) & t \leq t^* \\ F_0 & t > t^* \end{cases}$$
(8.23)

The comparison is made for the case presented in fig. 4. For the present study, we have chosen, $\chi=4/t^*$, $t^*=20$. The time-averaged value of $\beta(t)$, averaged over 40 periods of external field (from $t_m^*=20$ to $t_{max}=60$) turns out slightly higher than in the case of instantaneous switching on of the external field ($\langle \beta \rangle \approx 0.78$). The probability distribution varies slightly, but also indicates less intensive excitation of the levels in the vicinity of n_0 and n_0+1 . Also the ionization probability does not change significantly ($P_{\Sigma} \approx 0.79$). On the whole, the adiabatic switching on of field did not give rise to new effects, although the value of critical perturbation is slightly increased.

VII. CONCLUDING REMARKS

The numerical simulation shows that the behaviour of the hydrogen atom under the influence of a periodic impulsive field, treated quantum mechanically differs from the behaviour emerging out of a corresponding classical calculation. The differences persist even in regions of the large quantum numbers, n >> 1. The presence of ionization due to direct coupling of the discrete basis to ionization channels is a quantum effect which has no corresponding analog in the classical system. In the quantum calculations, this ionization is caused by the presence of high frequencies in the external periodic delta function field. The calculations show that for strong perturbations an intense probability exchange between the neighboring states arises. However, in order to achieve the spreading seen in corresponding classical calculations, a substantially large $(F_{\text{quantum}} \approx 3F_{\text{classical}})$ strength is required in the quantum calculations. Nevertheless, in regarding the effects of direct ionization as irrelevant to the stochastic diffusion, we found that the excitation of the higher levels of hydrogen atom is still very restrictive compared to the diffusion emerging from the semi-classical calculations. Preliminary numerical experiments indicate that such a behaviour (apart from the strong direct ionization) is also a feature of the models with monochromatic external fields.

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A hypergeometric series F is a series of the form

$$+ \frac{\Lambda(\Lambda+7)(\Lambda+5) \cdot 7 \cdot 5 \cdot 3}{\gamma(\gamma+7)(\gamma+5)b(b+7)(b+5)} \stackrel{5}{=} _{3} + \cdots$$

$$+ \frac{\Lambda(\Lambda+7)(\Lambda+5) \cdot 7 \cdot 5 \cdot 3}{\gamma(\Lambda+7)(\rho+5)} \stackrel{5}{=} _{3} + \cdots$$
(1)

This series terminates if λ or β is equal to a negative integer or to zero. For $\lambda = -k$ (k = 0, 1, 2, ...), the hypergeometric series is intermediate if neither λ nor β is equal to $-\ell$ (where $\ell < k$ and ℓ is a natural number).

In equation (4.12) the hypergeometric series

$$F\left(-n_1,-q;-n_2-q-lml;\frac{b_{nn'}(b_{nn'}-d_n-d_{n'})}{(b_{nn'}-d_n)(b_{nn'}-d_{n'})}\right),$$
(2)

can be intermediate since the parameter $n_1+q+|m|$ can be zero (both n_1 and q range from zero to some value, and in our present calculations, m=0). To avoid this problem, we give below a proof of the transformation in which the hypergeometric series does not lead to indeterminancy. According to equation (1), we have for the series:

$$F(-k, \beta; \lambda; f) = f - \frac{\lambda(\lambda+1) \cdots (\lambda+k-1)}{k} \frac{K(k-1) \cdots (k-k+1) \dot{b}(k+1) \cdots (k+k-1)}{(\lambda+k-1)} \cdot \frac{K(k-1) \cdots (k+k-1)}{f} \cdot$$

Let.

$$F(-k,p;v;z) = C_0 F(-k,p;\delta;1-z)$$
 (4)

The coefficient of the highest power Zk/k! in eq. (4) is:

$$C_0 \frac{g(g+1)\cdots(g+k-1)}{g(g+1)\cdots(g+k-1)} = (-1)_k \frac{g(g+1)\cdots(g+k-1)}{g(g+1)\cdots(g+k-1)}, \qquad (5)$$

or:

$$C_{o} = \left(-1\right)^{k} \frac{S\left(S+1\right) \cdots \left(S+k-1\right)}{S\left(S+1\right) \cdots \left(S+k-1\right)}$$
(6)

Then, the coefficient of $Z^{k-1}/(k-1)$! is:

$$C_{0}(-1) = (-1)_{k-1} \frac{\lambda(\lambda+1)\cdots(\lambda+k-5)}{k' \cdot b(b+1)\cdots(b+k-1)} + (-1)_{k-1} \frac{\Sigma(2+1)\cdots(2+k-5)}{k' \cdot b(b+1)\cdots(b+k-5)}$$

$$(4)$$

Thus.

$$C_{0}(-1)_{\kappa} \left\{ \frac{2(2+1)\cdots(2+k-5)}{2(2+1)\cdots(2+k-5)} \cdot (2+k-5) \right\}$$

$$= \frac{\kappa_{1} b(b+1)\cdots(2+k-5)}{2(2+k-5)\cdots(2+k-5)} \cdot (2+k-5)$$
(8)

or

$$C_{o} = \left(-1\right)^{k} \frac{\delta(\delta+1)\cdots(\delta+k-1)}{\delta(\delta+1)\cdots(\delta+k-1)(\beta-\delta)}$$

Comparing eqs. (9) and (6), we obtain

or,

$$C_0 = (-1)^k \frac{(\beta - \nu) \cdots (\beta - \nu - k + 1)}{(\beta - \nu) \cdots (\beta - \nu - k + 1)}.$$
(10)

As a result, we have the relation:

$$= \frac{(-1)^{k}(\beta-\nu)(\beta-\nu-k+1)}{\nu(\nu+k)} F(-k,\beta;\beta-\nu-k+1;1-2).$$
(11)

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Figures Captions

- Fig. 1. Dependence of the probability on time $P_n(t)$ for the weak field; $n_0 = 7$; $F_0 = 0.0015$; T = 2627; $\xi = 0.0027$.
- Fig. 2. Dependence of the probability P_n on time for two states $|n_0 = 9\rangle$ and $|n = 10\rangle$. The initially populated state is $N_1 = N_2 = 4$, with the parameters: $\frac{7}{5} \approx 0.005$, $\frac{7}{5} \approx 5357$, $\frac{1}{5} \approx 0.002$, $\frac{1}{5} \approx 300$; $\frac{1}{5} \approx 10.002$.
- Fig. 3. Coherent oscillations of the probability for $n_0 = 9(n_1 = n_2 = 4)$ under the different periods T; $F_0 = 0.008$, $t_m = 300$. a) $\xi \approx 0.026$, T = 4000; b) $\xi \approx 0.021$, T = 5000; c) and d) $\xi \approx 0.017$, T = 6000.
- Fig. 4. Coherent oscillations of the probability for the states $|n_0\rangle$ and $|n_0+i\rangle$ simultaneously with the strong direct ionization, $|n_0| = 9$, $|n_1| = 100$, $|n_2| = 100$, $|n_3| = 100$, $|n_4| = 100$, $|n_4|$
- Fig. 5. Coherent oscillations for the perturbation with main frequency, ω_o , which is above the threshold ω_{min} for direct ionization in a strong field: $N_o = 9$ ($N_1 = N_2 = 4$), $t_m = 300$, $t_m = 300$, $t_m = 400$, $t_m = 400$, $t_m = 400$, $t_m = 400$.
- Fig. 6. The probability of the direct ionization Pion versus time for the data of Fig. 5.
- Fig. 7. The probability distribution over different states with different n for no = 9 after t_m periods of external field; T = 5000. a) all parabolic states are initially populated for which \(\ext{t} = 0, \) \(\approx = 0.05, \) \(\int_0 = 0.01; \) b) only one parabolic state (\(n_1 = n_2 = 4 \)) is populated initially, \(\approx = 0.004, \) Fo = 0.008.
- Fig. 8. The probability dependence on the strength perturbation for the direct ionization ($\omega_o > \omega_{min}$) after periods $t_m = 1000$ is given; the number correspond to

- t=tm; no = 9 (n1 = n2), T=1000.
- Fig. 9. The typical behaviour for two resonant levels and empirical value of <β> (for the data of Fig. 4) on time t<tm = 40. The curves are the probabilities for the states |No = 97 and |N = 10 > correspondingly; curve 3 the dependence of β(t) (see (5.16); curve 4 the averaged quantity <β> for β(t); curve 5 the total probability P_ξ(t).
- Fig. 10. The total results for the dependence of <3> on perturbation \(\) for different initial states \(\n_0 \) with \(\bar{t} = 0 \), \(t_m = 40 \). The numbers indicate the principal numbers \(\n_0 = 9 \), 13, 17; the triangles correspond to \(\n_0 = 5 \).
- Fig. 11. The dependence of the total probability P_{Σ} (t_m=40) on ξ for different N_0 , notations are the same as for Fig. 10.

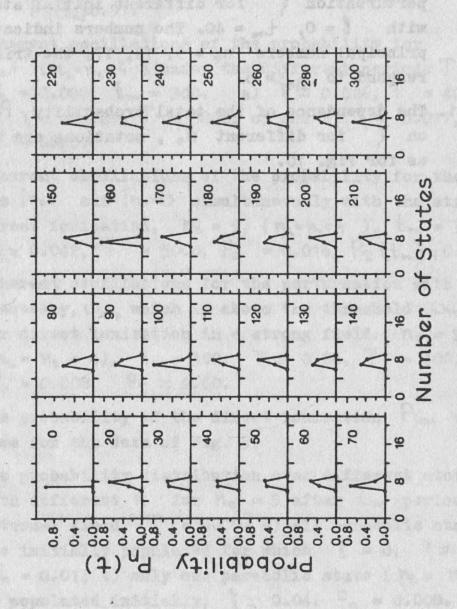


Fig. 1

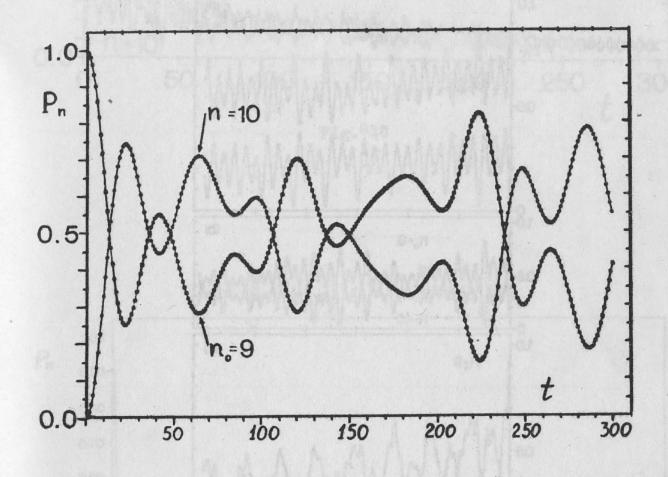


Fig. 2.

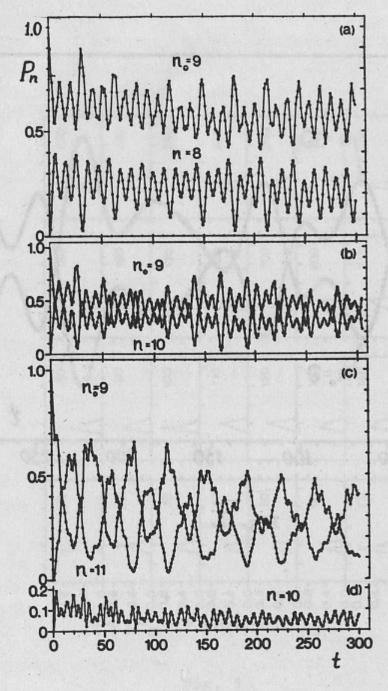
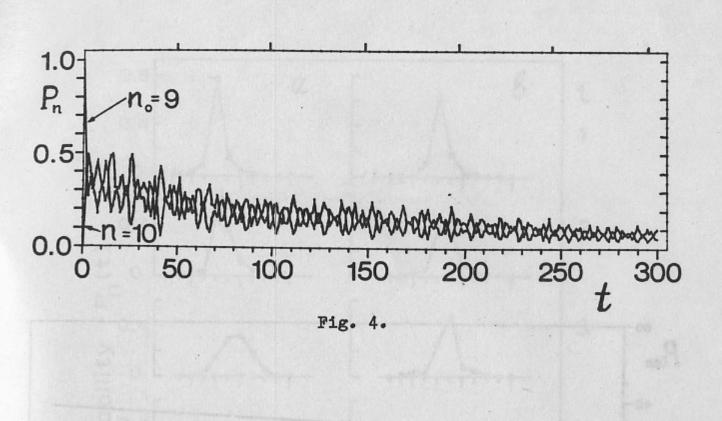
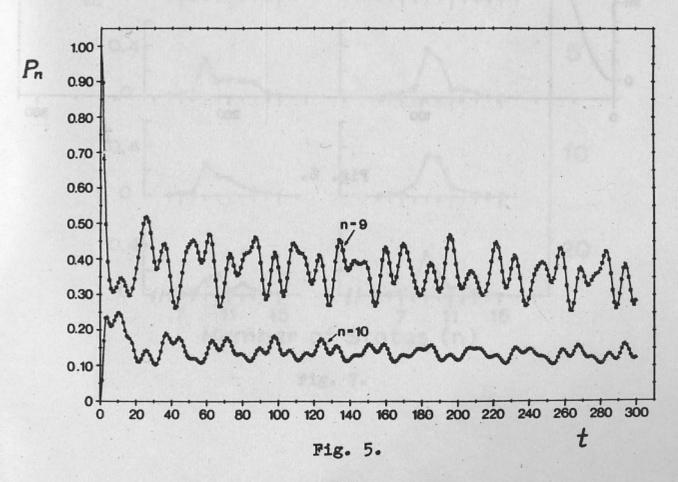
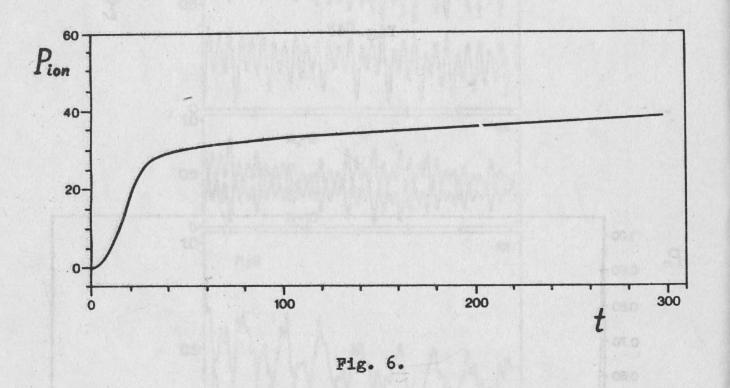


Fig. 3.







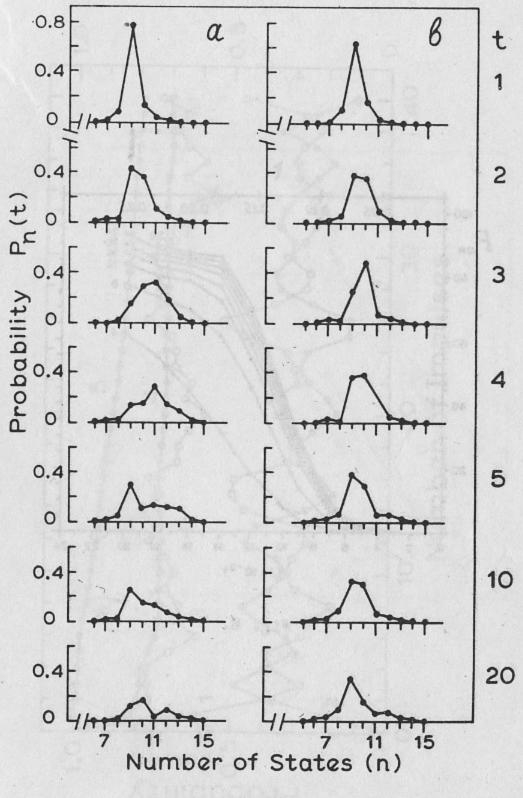
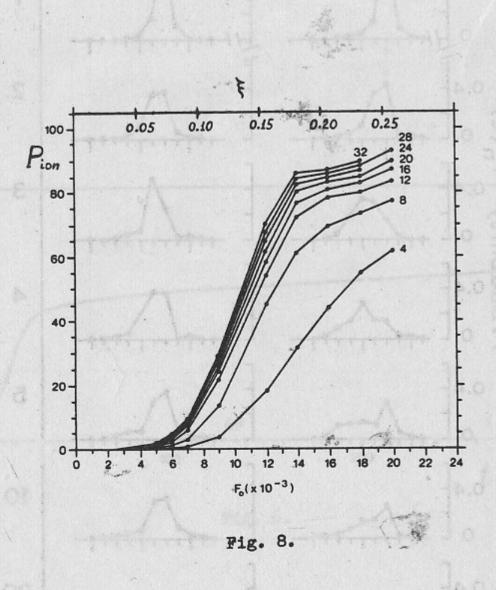
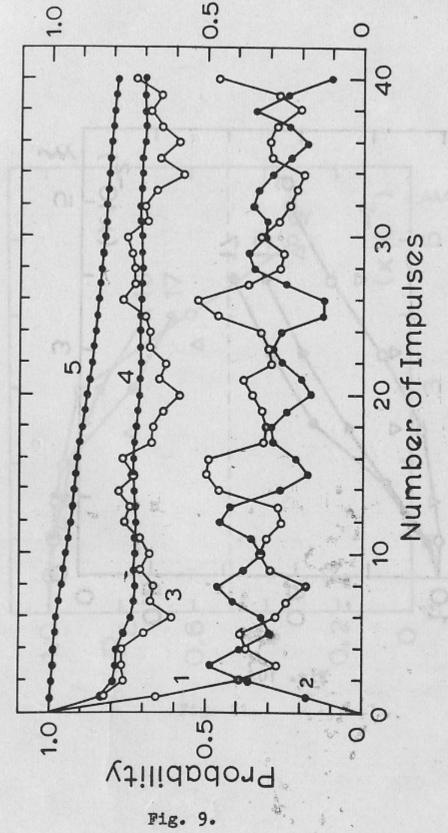
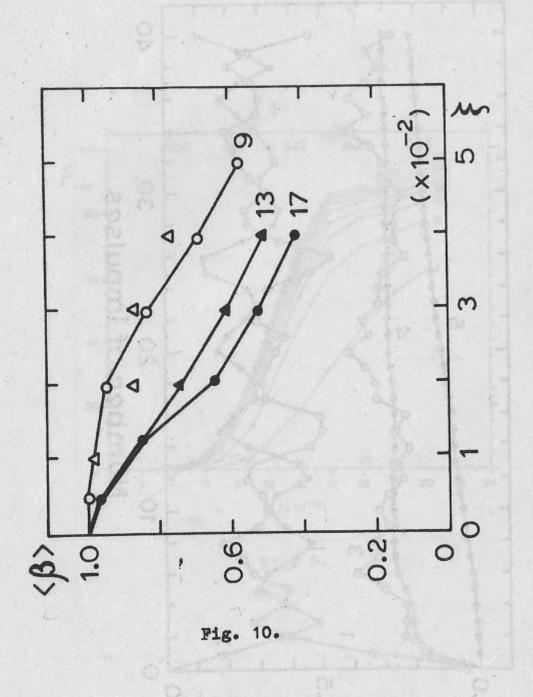


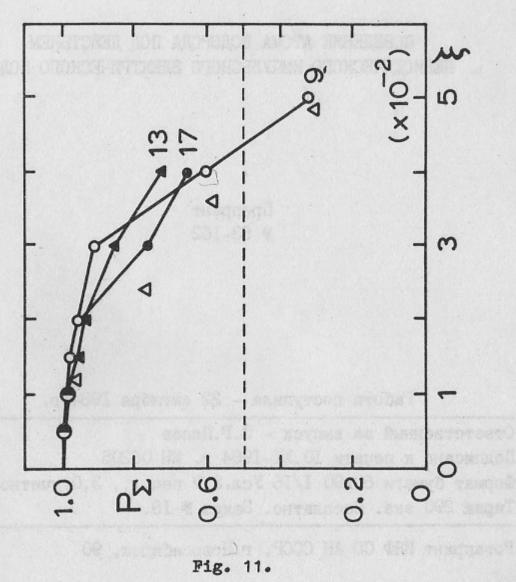
Fig. 7.



* FIE * F







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ПОВЕДЕНИЕ АТОМА ВОДОРОДА ПОД ДЕЙСТВИЕМ ПЕРИОДИЧЕСКОГО ИМПУЛЬСНОГО ЭЛЕКТРИЧЕСКОГО ПОЛЯ

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