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HYDROGEN IN MONOCHROMATIC FIELD: STABILIZATION AND CHANNELING VS. CHAOS

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ABSTRACT

The results of analytical and numerical investigations of classical atom in strong monochromatic linearly polarized electric field are presented. It is shown that the atom exhibiting fast chaotic ionization in small field becomes stable in the strong field limit. Analytical estimates for the dependence of the stabilization border on field frequency and projection of orbital momentum on field direction are obtained and compared with the results of numerical simulations. The analogy between stabilization and channeling of electrons in a crystal is established. Conditions for the observation of stabilization of Rydberg atoms in laboratory experiments are discussed.

INTRODUCTION

Since the pioneer experiment of Bayfield and Koch in 1974 [1] the problem of ionization of highly excited states of hydrogen atom in a monochromatic electric field attracts a great deal of attention (see [2] and Refs. there in). It happened that this system with quite simple equations of motion lies on the intersection of few modern lines of development in physics being the following: classical and quantum chaos, Anderson localization, multiphoton ionization, Rydberg atoms. Only the knowledge of the physics of these fields allowed to understand the origin of the fast ionization observed in the experiments. During the long time there was the impression [3] that due to high values of principal quantum number ($n_0 \sim 70$) the ionization process can be understood on the basis of classical equations of motion which give rise to classical chaos and fast diffusive excitation. However, the first theoretical investigations of quantum problem [4] showed that under certain conditions quantum effects can lead to localization of classical chaos and sharp suppression of ionization. Further researches allowed to find the quantum delocalization border above which ionization goes in a classical way and below which ionization probability is negligible in comparison with classical value [5]. The origin of this phenomenon can be understood on the grounds of the Kepler map description and analogy with the Anderson localization in solid state [6]. After that there was the impression that the physics of that system is mainly clear. However, recent results for stabilization of atom in strong field [7] showed that still there are many open questions. While in [7] the authors tried to analyse directly the quantum problem from my viewpoint the quantum analysis can be more successful at the second step after the understanding of the physics of classical atom in strong field. Some first results in that direction were announced in [8,9]. The analysis of classical stabilization, its applicability to the quantum case and its analogy with channeling of particles in a crystal will be the main subject of this talk.

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KEPLER MAP

The great improvement of the understanding of the process of ionization of excited states in hydrogen atom by a monochromatic linearly polarized field had been achieved on the grounds of one-dimensional atom model [2,4,6]. This model gives a good description of excitation not only for the states extended along the field direction [4] but also for the 3-dimensional states as it was shown in [6]. In the classical case the dynamics depends only on rescaled field strength $\epsilon_0 = \epsilon n_0{}^4$ and frequency $\omega_0 = \omega n_0{}^3$ (here and below we use atomic units, n_0 is the principal quantum number of initially excited level). The typical experimental conditions [1,2] correspond to $n_0 \approx 70$, $\epsilon_0 \approx 0.05$, $\omega_0 \approx 1$ so that up to 40-70 photons $N_I = n_0/2\omega_0$ are required to ionize one atom.

Numerical and analytical investigations of one-dimensional model showed that in the case of high microwave frequency ($\omega n^3 > 1$) the dynamics of the system, which originally is ruled by the continuous Hamiltonian equations, can be described by the Kepler map [6]:

$$\bar{N} = N + k \sin\phi, \quad \bar{\phi} = \phi + 2\pi\omega(-2\omega\bar{N})^{-3/2} \tag{1}$$

Here $k = 2.58\epsilon/\omega^{5/3}$, $N = E/\omega$ has the meaning of the number of absorbed or emitted photons (E is the energy of the electron), ϕ is the phase of microwave field at the moment when the electron passes near the nucleus. The bar denotes the new values of the variables after one orbital period.

The physical reason due to which the motion can be quite accurately [6] described by the simple area-preserving map is the following: when the electron is far from the nucleus microwave field leads only to a small fast oscillations which doesn't modify the average energy and the Coulomb trajectory of the electron. The change of energy happens only at perihelion where the Coulomb singularity leads to a sharp increase of the electron velocity. Ionization takes place when the energy of the electron becomes positive after a pass near the nucleus $N > 0$. Then the electron goes to infinity and never returns back. Therefore for the map (1) ionization is equivalent to absorption of trajectories with $N > 0$.

The Kepler map (1) can be locally reduced to the Chirikov standard map [10]. For that one needs to linearize the second equation in (1) near the resonant (integer) values of ωn^3 that gives:

$$\bar{N} = N + k \sin\phi, \quad \bar{\phi} = \phi + T\bar{N} \tag{2}$$

with $T = 6\pi\omega^2 n^5$. After quantization the variables (N, ϕ) become operators with commutation rule $[N, \phi] = -i$, the fractional part of N is constant and the system is locally equivalent to the quantized Chirikov standard map (quantum kicked rotator) [11]. Since in (2) global chaos takes place for $K = kT > 1$ we come to the conclusion that diffusive excitation in (2) takes place if $K = kT = 49\epsilon_0\omega_0{}^{1/3} > 1$. The diffusion rate is equal to $D = k^2/2$ and according to [11,6] the localization length for the steady-state distribution, measured in the number of photons, is equal to $l_\phi = D = 3.33\epsilon^2/\omega^{10/3}$. The difference from the localization length for a quasienergy eigenfunction where $l = D/2$ is connected with the strong fluctuations at the tail (see [11]). If the localization length is less than the number of photons required for ionization N_I then the ionization rate will be exponentially small: $W \sim \exp(-2N_I/l_\phi)$. In the opposite case $l_\phi = D > N_I$ the delocalization takes place and the process of ionization is close to the classical one. In the 3-dimensional atom the Coulomb degeneracy leads to a slow motion along energy surface that allows to describe the excitation in energy also by the Kepler map with a small change of constant k [6]. Numerical simulations with the quantum Kepler map [12] reproduce the 10%-threshold for ionization obtained in the laboratory [13]. Quantum suppression of classical chaotic ionization was also observed in the laboratory experiments with hydrogen [14] and rubidium [15] atoms.

STABILIZATION

Being very successful in the description of energy excitation the Kepler map, however, cannot be applied for the case of very strong field. Indeed, in its derivation it was assumed that the change of energy after one kick $k\omega$ is much larger than the energy of free oscillations $\epsilon^2/2\omega^2$. This gives the condition of applicability of the Kepler map picture [6]:

$$\epsilon << \epsilon_{ATI} \approx 5\omega^{4/3} \tag{3}$$

Let us note that this condition is independent on the initial state since n_0 doesn't enter directly in the expression for ϵ_{ATI}.

In the one-dimensional case for $\epsilon >> \epsilon_{ATI}$ a collision with the nucleus, being unavoidable, goes in a fast way like with an elastic wall leading to a prompt ionization [6]. In the two-dimensional case for zero magnetic quantum number m such collision also always takes place if the amplitude of free oscillations $\epsilon/2\omega^2$ is larger than the unperturbed distance between the electron and the nucleus in perihelion $l^2/2$ (l is the orbital momentum). This gives the condition of prompt ionization for $l > (3/\omega)^{1/3}$ [8]:

$$\epsilon > \omega^2 l^2/4 \tag{4}$$

where it was assumed that l is few times less than n. For $l < (3/\omega)^{1/3}$ ionization is ruled by the Kepler map and for $\epsilon_0 > {\omega_0}^{2/3}/2.6$ prompt ionization takes place after one orbital period (see (1)). Therefore, there is no stabilization of classical atom in the strong field for $m = 0$.

A qualitatively different situation arises for the case of non-zero projection of orbital momentum m on the field direction. For linear polarization the projection m is the exact integral of motion and it creates for the electron a possibility to avoid close collision with the nucleus. To analyse the motion in the strong field it is convenient to use an oscillating frame and cylindrical coordinates in which the Hamiltonian has the form:

$$H = \frac{{p_z}^2}{2} + \frac{{p_\rho}^2}{2} + \frac{m^2}{2\rho^2} - \frac{1}{(\rho^2 + (z - \frac{\epsilon}{\omega^2}\sin(\omega t))^2)^{1/2}} \tag{5}$$

If the frequency of the nuclear oscillations is large enough (the condition will be given later) then in first approximation the nucleus can be considered as a charged thread with a linear charge density σ slowly dependent on z: $\sigma(z) = \omega^2/(\pi\epsilon(1-(z\omega^2/\epsilon)^2)^{1/2})$. Then, for small z and ρ the Hamiltonian of averaged motion takes the form [9]:

$$H_{ave} = \frac{{p_z}^2}{2} + \frac{{p_\rho}^2}{2} + \frac{m^2}{2\rho^2} + 2\sigma(z)\ln(\frac{\rho\omega^2}{\epsilon}) \tag{6}$$

The constant under the logarithm takes into account that for $\rho >> \epsilon/\omega^2$ the coupling energy becomes much less than ω^2/ϵ. From (6) one easily finds the position of the potential minimum $\bar{\rho} = \sqrt{\pi\epsilon/2}m/\omega$ and the frequency of small oscillations $\Omega = 2\sqrt{2}\omega^2/(\pi\epsilon m)$ (for $z << \epsilon/\omega^2$). The depth of the potential or the energy required for ionization of atom is approximately $I \approx 2\omega^2 L/\pi\epsilon$ with $L = \ln(2\epsilon/(e\pi\omega^2 m^2))/2$. The minimal distance between the nucleus and electron is determined by the condition $I = m^2/2(\rho_{min})^2$ giving:

$$\rho_{min} = \frac{m}{2\omega}\sqrt{\frac{\pi\epsilon}{L}} \tag{7}$$

The physical reason for the growth of the minimal distance with the field strength is the following: with the increase of the field the amplitude of the field oscillations grows leading to the decrease of attractive Coulomb force while the centrifugal potential remains the same.

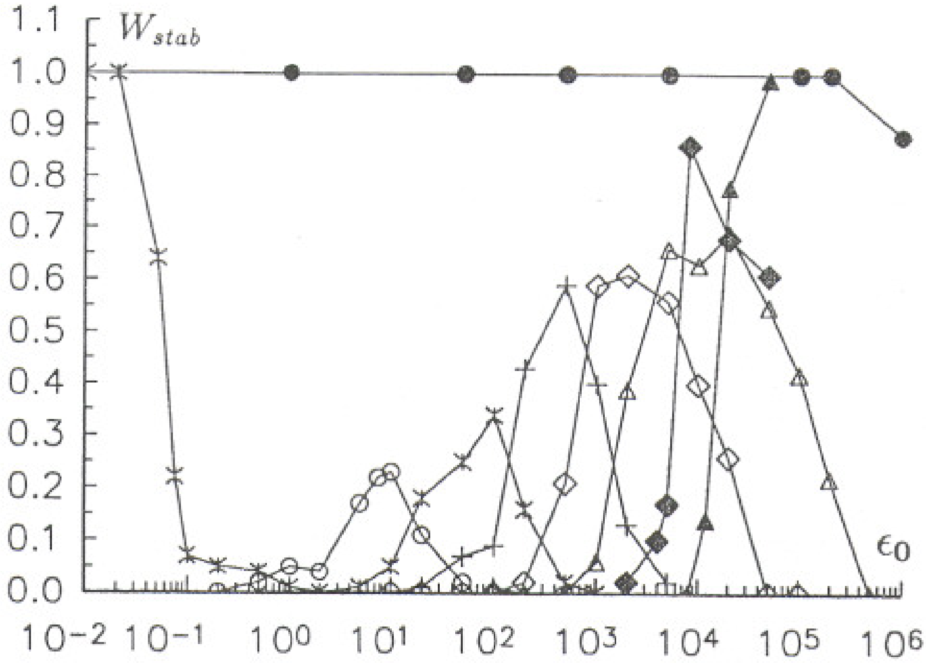
The averaged description of the motion (6) is correct if the frequency of field oscillations ω is much larger than the frequency Ω of oscillations in ρ. In that case the averaged Hamiltonian (6) is the constant of the motion with adiabatic accuracy and ionization of atom doesn't take place. This gives the stabilization border [9]:

$$\epsilon > \epsilon_{stab} = \alpha\frac{\omega}{m} \tag{8}$$

where α is some numerical constant. The same estimate can be obtained from the condition that the change of energy ΔE during the collision between the electron and the nucleus is smaller than I. Indeed, the change of the momentum is $\Delta p \approx \Delta t/{\rho_{min}}^2 \approx \omega/(\epsilon\rho_{min})$ and the change of the energy $\Delta E \approx \omega^2/(\epsilon^2{\rho_{min}}^2)$ is less than I if (8) is satisfied. Another condition intrinsically used in derivation of (6) and (8) is $\rho_{min} < \epsilon/\omega^2$ which gives $\epsilon > m^2\omega^2$. Also, there are two qualitatively different situations depending on the ratio between m and $(3/\omega)^{1/3}$. In the case $m << (3/\omega)^{1/3}$ (stabilized atom regime) we have $m^2\omega^2 << 5\omega^{4/3} << \alpha\omega/m = \epsilon_{stab}$. For small field amplitude (3) the excitation is described by the Kepler map and the complete ionization after one orbital period of the electron takes place for $\epsilon_0 > {\omega_0}^{2/3}/2.6$ [6]. Between this border and above chaos border $\epsilon_{c0} = 1/49{\omega_0}^{1/3}$ ionization goes in diffusive way which is also relatively fast. However, for the more strong field (8), when the Kepler map picture is not valid (see (3)), atom becomes stable. The case of opposite inequality is less impressive. Indeed, for $m >> (3/\omega)^{1/3}$ (stable atom regime) we have $\alpha\omega/m << 5\omega^{4/3} << m^2\omega^2$ and atom remains stable (nonionized) up to $\epsilon \sim m^2\omega^2$ as it was in (4) ($l \sim m$). Above this value a significant portion (order of half) of atoms will remain stable since condition (8) is satisfied. Finally, ionization takes place only when the value of ρ_{min} (7) becomes larger than the size of the atom $2{n_0}^2$ and the electron cannot be captured in the stable region during the switching of the field. This gives the destabilization border

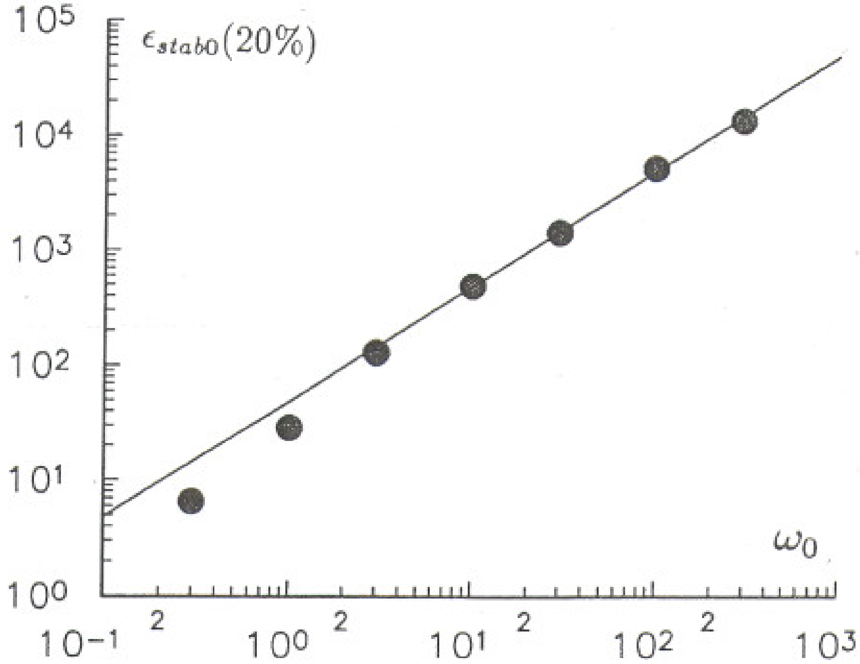
$$\epsilon_{destab} \approx \frac{16L\omega^2{n_0}^2}{\pi m^2} \tag{9}$$

This border is also valid for the case $m << (3/\omega)^{1/3}$. Of course, in that case the stabilization can be observed only for the time of field switching T_{sw} less or order of one orbital period of the electron. Otherwise a collision with nucleus will take place at field strength $\epsilon < \epsilon_{stab}$ and atom will be ionized.



1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
W_{stab}
ϵ_0
10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5} 10^{6}

Fig. 1



10^5
10^4
10^3
10^2
10^1
10^0
$\epsilon_{stab0}(20\%)$
ω_0
10^{-1} 10^{0} 10^{1} 10^{2} 10^{3}

Fig. 2

The results of numerical simulation of ionization process of system (5) are presented on the Fig.1. The stabilization probability $W_{stab} = 1. - W_{ion}$ is given for different field strengths ϵ_0 and frequencies (ω_0=0.3 (○), 1. (*), 3. (+), 10. (◇), 30. (△), 100. (◆), 300. (▲), 1000 (•)). The ionization probability W_{ion} was defined as the relative part of the trajectories with positive energies after field pulse. The initial distribution of 100 trajectories (25 for $\omega_0 = 1000.$) corresponded to a quantum state with fixed spherical quantum numbers (fixed actions and equipartition in conjugated phases). The initial value of orbital momentum was equal to l/n_0=0.3 and its projection was equal to m/n_0=0.25. The time of field switching (on/off) measured in the number of field periods was chosen to be equal to $T_{sw} = \omega_0$ (one unperturbed orbital period of the electron). The pulse duration of the field was $T_{int} = 500\omega_0$ (500 orbital periods). The data clearly demonstrate the stabilization of atom for field strength larger than some critical value. It is convenient to define the stabilization border as the field strength $\epsilon_{stab0}(20\%)$ for which $W_{stab} = 0.2$. The dependence of $\epsilon_{stab0}(20\%)$ on ω_0, extracted from the data of Fig.1, is presented on Fig.2. The numerical data (black points) are well described by the theoretical expression (8) with $\alpha = 12$ (straight line) in the wide frequency range. This dependence continues up to $\omega_0 = 1000$ where we enter in the stable atom regime with $m > (3/\omega)^{1/3}$ and where stabilization disappears in agreement with above theoretical arguments (see Fig. 1). However, the stability of atom in that case is of the other nature than it was in [8] since the condition (4) is strongly violated. So, for such strong fields stability of atom is based on the same physical grounds (8) as in the stabilized atom regime for $m << (3/\omega)^{1/3}$. The numerical check of the dependence of stabilization border $\epsilon_{stab0}(20\%)$ on m is presented on Fig.3 ($l/m = 1.2$) and also demonstrates good agreement with the theory (8) (numerical data are presented by points, straight line gives the theory (8) with $\alpha = 12$). However, some increase of ϵ_{stab} in comparison with (8) is visible for small m. So, it will be good to have a more detail investigation of this region (see also [9]).

Another characteristic feature of Fig.1 is the disappearance of stabilization for very high fields. The destabilization border $\epsilon_{destab0}(20\%)$ defined from Fig.1 by the condition $W_{stab} = 0.2$ (black points) is in satisfactory agreement with the analytical estimate (9) (full line) as it is seeing on Fig.4. Due to this destabilization atom can be captured in the stabilization regime only for the fields in the interval $\alpha\omega_0/(m/n_0) < \epsilon_0 < 16L\omega_0^2/(\pi(m/n_0)^2)$. Therefore, the minimum stabilization border for ϵ_0 is near 10. Let us note that it is possible to have stabilization even for $\omega_0 << 1$ (see Fig.1) if the momentum is small enough ($m/n_0 << \omega_0$). However, in that case the size of atom will be quite big (ϵ_0/ω_0^2) leading to a small coupling energy I.

Another interesting regime of motion appears in the limit of high frequencies and small m (ω_0 =100, 300 on Fig.1). In this case the amplitude of nuclear oscillations ϵ/ω^2 is much less than the size of unperturbed atom $2n_0^2$ and ionization energy is practically the same as for unperturbed case. Numerical simulations shows that the size of the atom remains comparable with the unperturbed one during many orbital periods of the electron. Examples of two trajectories for such case are presented on Fig. 5 ($\omega_0 = 100$, $\epsilon_0 = 8000$) and Fig. 6 ($\omega_0 = 300$, $\epsilon_0 = 20000$) with initial $l/n_0 = 0.3$ and $m/n_0 = 0.25$. In both cases 10^5 field periods are shown. In these cases the significant change of the size of the orbits clearly shows that the average energy is not conserved. Probably the motion is chaotic

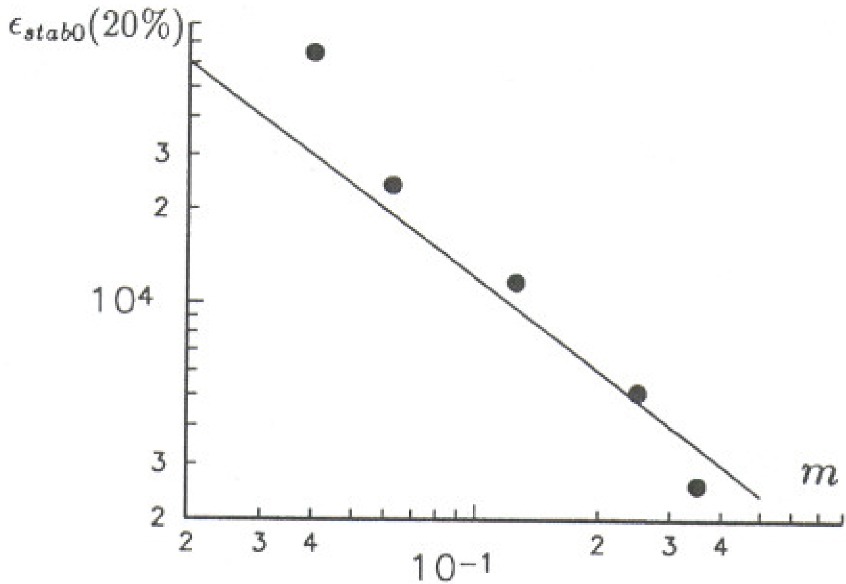

$\epsilon_{stab0}(20\%)$
3
2
10^4
3
2
m
2
3
4
10^{-1}
2
3
4

Fig. 3

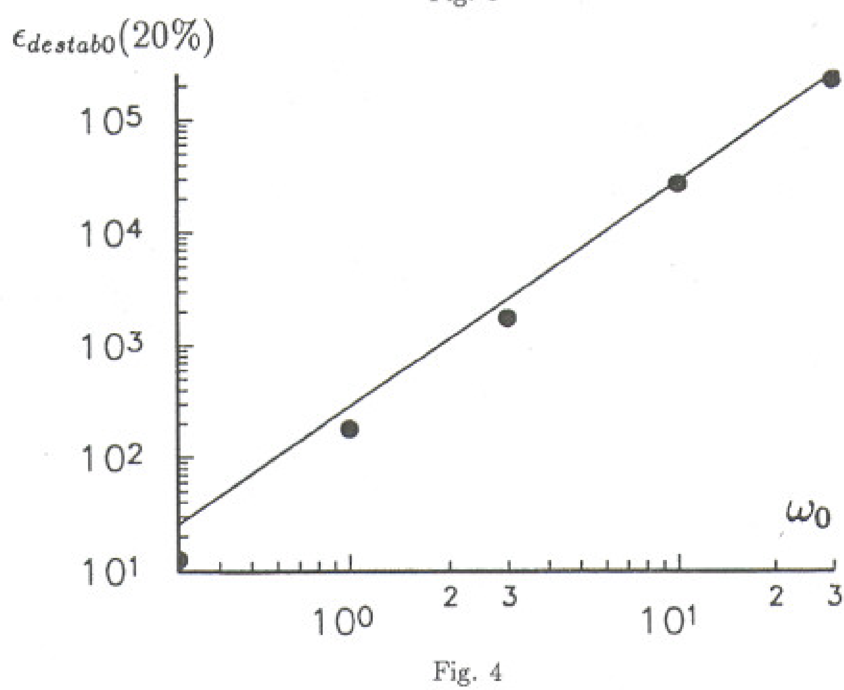

$\epsilon_{destab0}(20\%)$
10^5
10^4
10^3
10^2
10^1
ω_0
10^0
2
3
10^1
2
3

Fig. 4

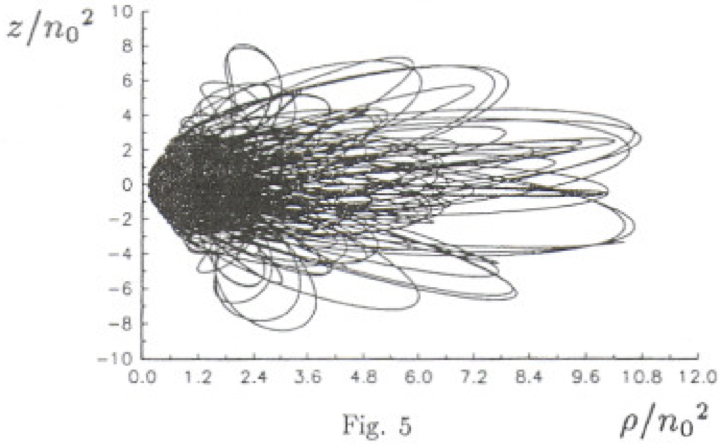


Fig. 5

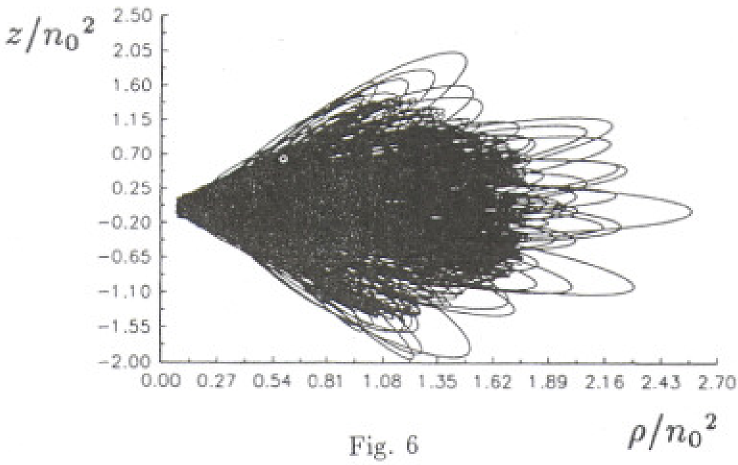


Fig. 6

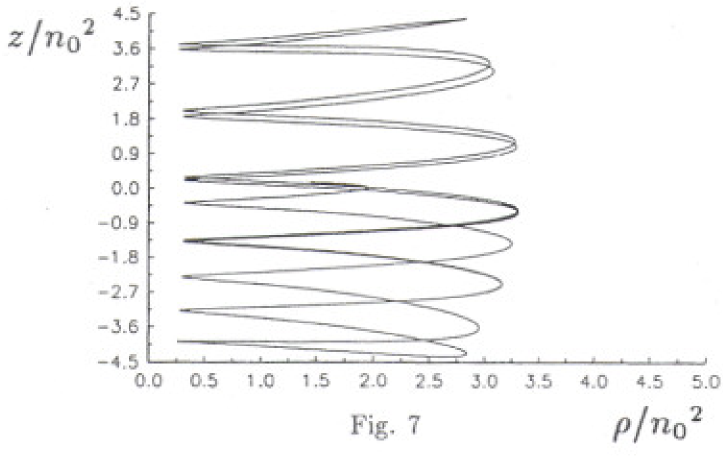


Fig. 7

and after many many periods the orbits will be ionized. However, it is necessary to develop a new theory for description of this process since the field is much stronger than (3) and the Kepler map picture cannot be applied. In spite the fact that $\epsilon/\omega^2 << n_0^2$ the condition $\rho_{min} << \epsilon/\omega^2$ is satisfied and the stabilization border is still given by (8) that is confirmed by the data of Fig. 2. An example of regular motion in the stable atom regime ($m >> (3/\omega)^{1/3}$) is presented on Fig. 7 for $\omega_0 = 1000$, $\epsilon_0 = 5\,10^6$, $m/n_0 = 0.25$, $l/n_0 = 0.3$, 50000 field periods with switching are shown.

CHANNELING ANALOGY

Here I would like to discuss the analogy between the phenomenon of stabilization of atom in strong field and the channeling of particles in a crystal (see for example [16] and Refs. there in). Let's consider the electron moving in the crystal with the velocity $v \approx c = 137$ (we will consider nonrelativistic case). Then in the frame of the moving electron its interaction with the protons in the crystal lattice will have approximately the form (5) if to take into account the interaction only with a nearest proton. On the grounds on that analogy we find that the effective distance between atoms in the crystal a and the velocity of the electron are equal to:

$$a = \frac{\epsilon}{\omega^2},\ v = \frac{\epsilon}{\omega} \tag{10}$$

The frequency of perturbation is $\omega = v/a$ so that $\epsilon = v^2/a$. Since in the crystal the distance between the atoms is approximately the same in all directions the analogy is valid for $\epsilon/\omega^2 > n_0^2$. The necessary condition of channeling is that the critical injection angle θ must be much less than one that implies: $\theta \approx v_\perp/v \approx 1/(v\sqrt{a}) \approx (\omega^{4/3}/\epsilon)^{3/2} << 1$. This is the condition of unapplicability of the Kepler map (3). From the stabilization condition (8) it follows that channeling takes place for electrons with momentum $m > 10/v$. This is always satisfied for fast electrons with $v \approx 137$. The existence of channeling for very energetic electrons (that corresponds to strong field for stabilization problem) gives one more evidence for existence of stabilization of atom in strong field. Since high frequency radiation can be obtain from the channeling of relativistic electrons [16] it will be interesting to analyse the behavior of atom in so strong field that the motion of electron is relativistic. On the basis of the above analogy it is possible to expect strong radiation in the case of relativistic stabilization.

CONCLUDING REMARKS

In conclusion I would like to discuss the possibilities of observation of stabilization in laboratory experiments. In the first order this puts the question about the applicability of the above classical stabilization picture to the real quantum atom. The necessary condition discussed in [9] is that the number of photons required for ionization in (6) is much larger than one ($I >> \omega$). However, on the grounds of the channeling analogy this condition seems to be too restrictive. Indeed, channeling takes place even when the motion in the direction perpendicular to propagation is purely quantum and when the frequency $\omega = v/a$ is much greater than the coupling energy. The reason for that bases on the adiabaticity of the averaged motion which gives exponentially small Fourier components for high frequencies (or small matrix elements for transitions into continuum). Therefore, the stabilization will also take place in the quantum case if the conditions (8)-(9)

are satisfied. However, the motion can be of a purely quantum nature if the low levels in the averaged potential (2) are excited. According to (8),(9) for $n_0 >> 1$ and $m \sim 1$ it is possible to have the energy of electron oscillations $(\epsilon/\omega)^2/2 >> 1$ even for $\epsilon << 1$ and $\omega << 1$. In this case the energy of the ground state is approximately the same as in the unperturbed case and therefore such stable (or long living) atom can radiate photons with the energy much greater than 13 ev during the radiative transition to the ground state. In the quantum case with $m = 0$ it is natural to expect that the stabilization border will be of the same order as for $m = 1$ giving $\epsilon_{stab} \sim 10\,\omega$. For $n_0 = 30$ and the frequency of CO_2 laser ($\omega \sim 1/300$, $\omega_0 \approx 100$) the stabilization border ϵ_{stab} will change in the interval $2\,10^8$ to 10^7 V/cm for the change of m from 1 (or 0) to 15.

Of course, future investigations are required for a better understanding of the stabilization both in the classical and quantum cases.

I would like to thank Professor H.Walther for the stimulating interest to my chaotic researches of Rydberg atoms.

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