Ionization of Rydberg atoms in a low frequency field: modelling by maps of transition to chaotic behavior

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Abstract. We investigate a microwave ionization of highly excited atom in a low frequency field and show that such a process may be studied on the bases of map for the electron energy change during the period of the electron motion between two subsequent passages at aphelion. Simple approximate criterion results to the threshold field for transition to chaotic behavior very close to the numerical results. We show that transition from adiabatic to chaotic ionization mechanism takes place when the field frequency to the electron’s Kepler frequency ration approximately equals 0.1.

1. Introduction

Highly excited atom in a monochromatic field is one of the simplest real strongly driven by an external driving field nonlinear system with stochastic behavior. That is why recently a large amount of effort, both theoretical and experimental, has been devoted to the studies of the Rydberg atoms in strong microwave fields (for review see [1-3] and references therein). The observation of excitation and ionization rates provides evidence for stochastic behavior of weakly bound electron: the ionization of Rydberg atoms exhibits a threshold dependence on the field amplitude and, at least for the low relative frequency of the field, appears as a diffusion like process. The classical dynamics of the excited electron may be described by the map, called the ”Kepler map”, rather than by differential equations of motion [4,5], which greatly facilitates the numerical and analytical investigation of stochasticity and ionization process. The map, mostly represented for the number of absorbed photons, is widely used for the analysis of chaotic processes for relatively high frequencies of the field [1-5]. In the very low frequency region the ionization is direct: the electron escapes over the potential barrier [5-6]. However, the threshold field for the direct low frequency (adiabatic) ionization is considerably higher than that for the transition to chaotic behavior in the medium and high frequency field. On the other hand, the derivation of the mapping equations of motion [4,5] is based on the classical perturbation theory. Therefore, the question of the validity of these maps for description of the ionization process in the low frequency relatively strong field arises. In addition, the transition from adiabatic to chaotic ionization mechanism is of great interest, especially as the classical ionization theory is proper for the low frequency ionization.

It is the purpose of this work to investigate the fitness of the classical maps [4,5] for the low-frequency ionization of Rydberg atoms and on this basis to analyse a transition from adiabatic to chaotic motion in the strongly driven by the slow external field system.
2. Equations of motion and dynamics

The direct way of coupling the electromagnetic field to the electron Hamiltonian is through the $\mathbf{A} \cdot \mathbf{P}$ interaction, where $\mathbf{A}$ is the vector potential of the field and $\mathbf{P}$ is the generalized momentum of the electron. Thus the Hamiltonian of the hydrogen atom in a linearly polarized field $F \cos(\omega t + \vartheta)$, where $F$ and $\omega$ are the field strength amplitude and frequency, in atomic units has the form

$$H = \frac{1}{2} \left( \mathbf{P} - \frac{F}{\omega} \sin(\omega t + \vartheta) \right)^2 - \frac{1}{r}. \quad (1)$$

The electron energy change due to the interaction with the external field follows from the Hamiltonian equations of motion [7]

$$\dot{E} = -\dot{r} \cdot F \cos(\omega t + \vartheta). \quad (2)$$

Measuring the time of the field action in the field periods one can introduce the scale transformation [8] when the scaled field strength and energy are $F_s = F/\omega^{4/3}$, and $E_s = E/\omega^{2/3}$. However, it is convenient to introduce the positive scaled energy $\varepsilon = -2E_s$ and relative field strength $F_0 = Fn_0^4 = F_s/\varepsilon_0^2$, with $n_0$ being the initial principal quantum number.

Note, that eq. (2) is exact if $\dot{r}$ is obtained from the equations of motion including the influence of the electromagnetic field. Using the parametric equations of motion we can calculate the change of the electron’s energy in the classical perturbation theory approximation. We restrict our subsequent consideration to the one-dimensional model, which corresponds to the states with low orbital quantum numbers $l \ll n$. The integration of eq. (2) for the motion between two subsequent passages at the aphelion (where $\dot{x} = 0$ and there is no energy change) results to the map (see [4,5] for details)

$$\begin{aligned}
\varepsilon_{j+1} &= \varepsilon_j - 4\pi F_0 \frac{\varepsilon_j^{5/2}}{\varepsilon_{j+1}^{5/2}} J_{s_j+1}(s_{j+1}) \sin \vartheta_j \\
\vartheta_{j+1} &= \vartheta_j + 2\pi \varepsilon_j^{-3/2} + G(\varepsilon_{j+1}, \vartheta_j)
\end{aligned} \quad (3)$$

where $s = \varepsilon^{-3/2} = \omega/(-2E)^{3/2}$ is the relative frequency of the field, $J'_s(z)$ is the derivative of the Anger function and function $G$ may be obtained from the requirement of area-preserving [4]. In the low frequency $s \ll 1$ limit $J'_s(s) \simeq s/2$ and we have the map

$$\begin{aligned}
\varepsilon_{j+1} &= \varepsilon_j - 2\pi F_0 \left( \frac{\varepsilon_j^2}{\varepsilon_{j+1}^{5/2}} \right) \sin \vartheta_j \\
\vartheta_{j+1} &= \vartheta_j + 2\pi \varepsilon_j^{-3/2} + 5\pi F_0 \left( \frac{\varepsilon_j^2}{\varepsilon_{j+1}^{7/2}} \right) \cos \vartheta_j
\end{aligned} \quad (4)$$

The results of the numerical analysis of maps (3) and (4) in the low frequency, $s \leq 1$, limit are presented in Fig. 1 and 2. We see that the threshold ionization field approaches the static field ionization threshold $F_0^{\text{st}} \approx 0.13$ when $s_0 \to 0$ ($\varepsilon \to \infty$). Thus, the maps (3) and (4) are valid in the low frequency limit when the strength of the driving electric field is of the order of the Coloumb field.

For the low frequencies, $2\pi s = 2\pi/\varepsilon^{3/2} \ll 1$, the change of the angle $\vartheta$ after one step of iteration is small and we can transform the system of equations (4) to the differential
Fig. 2. The relative threshold field strengths for the ionization outset from the numerical analysis of the maps (3) and (4) and according to the approximate criterion (8)-(9).

The relative threshold field strengths for the ionization outset from the numerical analysis of the maps (3) and (4) and according to the approximate criterion (8)-(9) equation

\[
\frac{d(\cos \vartheta)}{d\varepsilon} = \frac{\varepsilon}{\varepsilon_0 F_0} + \frac{5 \cos \vartheta}{2\varepsilon}.
\tag{5}
\]

The analytical solution of eq. (5) with the initial conditions \(\varepsilon = \varepsilon_0\) when \(\vartheta = \vartheta_0\) is

\[
\cos \vartheta = z^5 \cos \vartheta_0 - \left(\frac{2}{F_0}\right) z^4 (1 - z), \quad z = \sqrt{\varepsilon/\varepsilon_0}
\tag{6}
\]

For the relatively low values of \(F_0\) there is a motion in all the interval \(0 \div 2\pi\) of the angle \(\vartheta\). However for \(F_0 = 2z^4/5\) the increase of \(\vartheta\) at \(\vartheta \simeq \pi\) changes to the decrease and results to the fast decrease of \(\varepsilon\) and ionization process. The minimal value of \(F_0\) for such a motion corresponds to \(\vartheta_0 = 0\) and may be defined as a maximal value of \(F_0\) resulting to the motion in the interval \(0 \div 2\pi\), i. e., the maximum of the expression

\[
F_0 = 2z^4(1 - z)/(1 + z^5).
\tag{7}
\]

Such a maximum is at \(z = z_0\), where \(z_0\) is a solution of equation \(z^5 + 5z - 4 = 0\), i. e., \(z_0 = 0.75193\) and results to the \(F_0^0 = 0.1279\) which is only 1% lower the adiabatic ionization value \(F_0^{\text{ad}} = 2^{10}/(3\pi)^4 \simeq 0.1298\).

The approximate criterion for transition to chaotic behavior is [5]

\[
K = \max |\delta \vartheta_{j+1}/\delta \vartheta_j - 1| \geq 1
\tag{8}
\]

and according to eqs. (4) yields to the expression for the threshold field strength

\[
F_0^c = \varepsilon^5/6\pi^2 \varepsilon_0^2 = z_0^{10}/6\pi^2 s_0^2.
\tag{9}
\]
where $z_c$ is the solution of eq. (7) with $F_0 = F_c^0$. Note that $z_c^{10} \approx 1 - 10F_0^c + 30(F_0^c)^2 + \ldots$ if $F_0^c \leq 0.1$. For $0.09 \leq s_0 \leq 0.5$ expression (9) gives the ionization threshold field very close to the numerical results (see Fig. 2).

3. Conclusion

From the above analysis we can conclude that the map at aphelion (3) is suitable for the investigation of transition to chaotic behavior and ionization of Rydberg atoms also in the low frequency field, even for adiabatic ionization, when the strength of the external field is comparable with the Coloumb field. For such a purpose there is no need to use the map for the two halves of intrinsic period [9]. Moreover, the approximate criterion (8) for transition to chaotic behavior yields to the threshold field strength very close to the numerical results if we take into account the increase of the electron’s energy by the influence of the electromagnetic field. The transition from adiabatic to chaotic ionization occurs at the relative field frequency $s_0 \approx 0.1$.

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Fig. 1. Trajectories of the map (3) for the different initial conditions $\varepsilon_0, \theta_0$ and relative field strength $F_0$. The pictures in the left-hand side correspond to the regular quasiperiodic motion, while in the right-hand side represent the ionization process for a little bit stronger field. At $\varepsilon_0 \approx 4.3$, i. e. at $s_0 \approx 0.11$ the transition from the adiabatic to the chaotic ionization mechanism takes place.
From the map (3)

From the map (4)

According to eq. (9)