DIFFUSIVE IONIZATION OF RELATIVISTIC HYDROGEN-LIKE ATOM

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Abstract

Stochastic ionization of highly excited relativistic hydrogenlike atom in the monochromatic field is investigated. A theoretical analysis of chaotic dynamics of the relativistic electron based on Chirikov criterion is given for the cases of one- and three-dimensional atoms. Critical value of the external field is evaluated analytically. The diffusion coefficient and ionization time are calculated.

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Introduction

Investigation of properties of the highly excited atoms interacting with microwave field is important problem lying at the intersection of several lines of contemporary research. One of the important themes is chaos. Recently chaotic dynamics of atoms in the microwave fields have been subject of extensive research. Much theoretical and experimental work was devoted to this problem [1, 2, 3]. A theoretical analysis of behaviour of classical hydrogen atom, based on the Chirikov criterion [2, 4] shows that for some
critical value of field strength, the electron enters a chaotic regime of motion, marked by unlimited diffusion leading to ionization. Up to now much of the discussion on resonance overlap and chaos has largely been limited by nonrelativistic systems. It has been known, however, that chaotic dynamics can also be exhibited by systems undergoing relativistic motion \[11\]–\[14\] such as electrons in the free electron laser and driven relativistic electron plasma wave, driven relativistic oscillator and relativistic electron in the field of two Kepler centers.

As is well known, \[8, 9\] in the case of hydrogen atom interacting with strong enough (though still \(\varepsilon \ll \varepsilon_{cr}\)) monochromatic wave with \(\Omega \sim \omega_o = n^{-3}\) nonlinear oscillations of the atomic electron become stochastic, that leads to the diffusive ionization of the atom. Diffusion in the system arises due to the nonlinearity of the classical equations of motion. First mechanism of diffusive ionization was considered in \[15\]. The phenomenon of diffusive ionization was detected in the numerical experiments in \[16\]. The difference between diffusive ionization and other ones is the fact that in this case diffusive excitation corresponds to the increasing of energy of classical electron from the initial value to the ionization one.

In this paper we investigate the transition to chaos in the motion of a relativistic electron bound in the Kepler field under the influence of periodic external field. We generalize the above results on chaotic ionization of the classical nonrelativistic hydrogen atom to the cases of classical one- and three-dimensional relativistic hydrogen-like atom. As is well known (see \[8\]) and references therein), in the nonrelativistic case one of the remarkable features of the comparison of the classical theory with the experimental measurements of microwave ionization is the fact that a one-dimensional model of a hydrogen atom in an oscillating electric field pro-
vides an excellent description of experimental ionization thresholds for a real three-dimensional hydrogen atom. In the case of the relativistic hydrogenlike atom, one-dimensional model enables one to avoid the difficulties connected with the non-closeness of trajectories in the relativistic Kepler motion \cite{[17]} and the resulting additional degrees of freedom \cite{[18]}.

Using Chirikov’s criterion for stochasticity, we obtain, in terms of action and charge, the analytical formula for the critical value of microwave field at which stochastic ionization will occur. In this paper we will use the system of units $m_e = h = c = 1$ in which $e^2 = 1/137$.

**One-dimensional model**

Consider the classical relativistic electron in a field of one-dimensional $-\frac{Z\alpha}{x}$ potential where $Z$ is the charge of the center, and $\alpha = \frac{1}{137}$. The relativistic momentum of this electron is given by

$$p = \sqrt{(\varepsilon + \frac{Z\alpha}{x})^2 - 1},$$

where $\varepsilon$ is the full energy of the electron. The action is defined as

$$n = \int_{x_2}^{x_1} p \, dx = \frac{1}{\pi} a \sqrt{1 - \varepsilon^2},$$

where $a = \frac{\varepsilon Z\alpha}{1 - \varepsilon^2} x_1$ and $x_2$ are the turning points of the electron. From this expression the Hamiltonian is

$$H_0 = \frac{n}{\sqrt{n^2 + Z^2 \alpha^2}} \quad (1)$$

and the corresponding angular oscillating frequency is

$$\omega_0 = \frac{dH_0}{dn} = \frac{Z^2 \alpha^2}{(n^2 + Z^2 \alpha^2)^{3/2}} \quad (2)$$

It is easy to see that in the nonrelativistic limit (i.e., for small $Z$) both Hamiltonian and frequency coincide with corresponding nonrelativistic ones.
Now we consider interaction of our atom with monochromatic field which is written in the form

\[ V(x, t) = \epsilon \cos \omega t, \]  

where \( \epsilon \) and \( \omega \) are the field amplitude and frequency. First we need to write (3) in the action-angle variables. This can be done by expanding the perturbation (3) into a Fourier series:

\[ V(x, t) = \epsilon \sum_{-\infty}^{\infty} x_k(n) \cos(k \theta - \omega t), \]

where the Fourier amplitudes of the perturbation are defined by the integral

\[ x_k = \int_0^{2\pi} d\theta e^{im\theta} x(\theta, n) = -\frac{a}{k} J'(ek) = -\frac{n\sqrt{n^2 + Z^2\alpha^2}}{k} J'(ek), \]

\( J'_k \) is the ordinary Bessel function of order \( k \),

\[ e = \frac{\sqrt{n^2 + Z^2\alpha^2}}{n}. \]

Thus the full Hamiltonian of the relativistic hydrogenlike atom in the monochromotic field can be written in the form

\[ H = \frac{n}{\sqrt{n^2 + Z^2\alpha^2}} + \epsilon \sum_{-\infty}^{\infty} x_k(n) \cos(k \theta - \omega t). \]

For sufficiently small electric fields the Kolmogorov-Arnol’d-Moser theorem [10] guarantees that most of the straight-line trajectories in action-angle space will be only slightly distorted by the perturbation. The maximum distortion of the orbits will occur at resonances where the phase, \( k \theta - \omega t \), is stationary [10]. The resonance frequency and actions are therefore determined by the relation

\[ k \omega_0 - \omega = 0 \]
Then using Eqs. (2) and (7) the action resonant with the $k$th subharmonic of the perturbation is

$$n_k = \left[\left(\frac{kZ^2\alpha^2}{\omega^2}\right)^\frac{2}{3} - Z^2\alpha^2\right]^\frac{1}{2}$$  \hfill (8)

As is well known there are several methods for investigating the chaotic dynamics of a system with Hamiltonian in the form (3). Simplest of them is one, developed by Zaslavsky and Chirikov [4, 5, 7] which is called Chirikov criterion. According to this criterion chaotical motion occurs when two neighbouring resonances overlap i.e., when the following condition is obeyed:

$$\frac{\Delta n_k}{\delta n_k} > 1,$$  \hfill (9)

where $\Delta n_k$ is the width of $k$th resonance, $\delta n_k = n_{k+1} - n_k$ is the separation of the $k$ and $k+1$ resonances. Using (8) this separation is

$$\delta n_k = \left(\frac{kZ^2\alpha^2}{\omega}\right)^\frac{2}{3} \frac{1}{3kn_k}$$

According to [7, 10] the width of $k$th resonance defined as

$$\Delta n_k = 4\left(\frac{\epsilon x_k}{\omega'_0}\right)^\frac{1}{2}$$  \hfill (10)

where

$$\omega'_0 = \frac{d\omega_0}{dn} = \frac{3n_kZ^2\alpha^2}{(n_k^2 + Z^2\alpha^2)^\frac{5}{2}}.$$  

Note that these formulas for $\Delta n_k$ and $\delta n_k$ in the limit of small $Z$ coincide for known formulas corresponding to nonrelativistic case [1].

Taking into account the expression for $a$ and using the asymptotic formula $k^{-1}J'_k(ek) \approx 0.411k^{-\frac{5}{3}}$ (for $k \gg 1$) for the resonance width we obtain

$$\Delta n_k \approx \epsilon k^{-\frac{2}{3}}(Z\alpha)^{-3}(n_k^2 + Z^2\alpha^2)^\frac{1}{2}$$

Inserting expressions for $\Delta n_k$ and $\delta n_k$ into (9) we have

$$\epsilon^{\frac{1}{2}}k^{-\frac{1}{3}}(Z\alpha)^{-\frac{8}{3}}n_k(n_k^2 + Z^2\alpha^2)^\frac{1}{2} > 1$$
This gives us the critical value of the field amplitude at which stochastic ionization of the relativistic electron binding in the field of charge $Z\alpha$ will occur:

$$\epsilon_{cr} = k\frac{2}{3}(\pi Z\alpha)^3 n_k^{-2}(n_k^2 + Z^2\alpha^2)^{-1}$$

For small $Z$ the last formula can be expanded into series as follow:

$$\epsilon_{cr} = k\frac{2}{3}(Z\alpha)^3 n_k^{-4}(1 - \frac{Z^2\alpha^2}{n_k^2} + ...)$$

or

$$\epsilon_{cr} = \epsilon_{nonrel}(1 - \frac{Z^2\alpha^2}{n_k^2} + ...) \quad (11)$$

where $\epsilon_{nonrel}$ is the critical field corresponding to the nonrelativistic case.

As seen from this formula the critical field required for stochastic ionization of relativistic hydrogen-like atom is less than the corresponding nonrelativistic one.

**Three-dimensional model**

Hamiltonian of the relativistic electron moving in the Coulomb field in terms of action-angle variables can be written as [18]

$$H_0 = [1 + \frac{Z^2\alpha^2}{(n - M + \sqrt{M^2 + Z^2\alpha^2})^2}]^{-\frac{1}{2}}, \quad (12)$$

where $n = I_r + I_\phi + I_\theta$, $M = I_\phi + I_\theta$.

$I_r, I_\phi, I_\theta$ are the radial and angular components of the action.

For

$$M \gg Z\alpha = \frac{Z}{137} \quad (13)$$

this Hamiltonian can be rewritten as

$$H_0 = [1 + \frac{Z^2\alpha^2}{(n - M + M)^2}]^{-\frac{1}{2}} \approx \frac{n}{\sqrt{n^2 + Z^2\alpha^2}}. \quad (14)$$
The form of this Hamiltonian coincides with the one-dimensional Hamiltonian obtained in previous section. The frequency is defined by

$$\omega_0 = \frac{dH_0}{dn} = \frac{Z^2\alpha^2}{(n^2 + Z^2\alpha^2)^{\frac{3}{2}}}$$  \hspace{1cm} (15)

Consider now (following [9]) interaction of this relativistic three dimensional atom with external periodic field. Then the full Hamiltonian has the form

$$H = H_0 + \epsilon a e \cos \omega t \left[-\frac{3}{2} e \sin \phi + 2 \sum (x_k \sin \psi \cos k\lambda + y_k \cos \psi \sin k\lambda)\right],$$ \hspace{1cm} (16)

where

$$a = \frac{n}{Z\alpha} \sqrt{n^2 + Z^2\alpha^2}$$

$w$ is the frequency of external field. To obtain $x_k$ and $y_k$ in the relativistic case we consider trajectory equation of a relativistic electron in a Coulomb field [17]:

$$p + e \cos q \Phi = 1,$$ \hspace{1cm} (17)

where

$$p = \frac{M^2 - Z^2\alpha^2}{EZ\alpha}, \quad q = \sqrt{1 - \frac{Z^2\alpha^2}{M^2}}, \quad e = \frac{\sqrt{E^2M^2 - (M^2 - Z^2\alpha^2)}}{EZ\alpha},$$ \hspace{1cm} (18)

where $E$ - energy of the electron.

Due to the factor $q$ trajectory of motion of a relativistic electron in the Coulomb field is not closed [17]. If the conditions (13) and $q \approx 1$, $p \approx \frac{M^2}{E(Z\alpha)}$, are obeyed $e = \sqrt{1 - E^2}$. Therefore eq.(17) can be rewritten as

$$p + e \cos \Phi = 1,$$ \hspace{1cm} (19)

Then for the Fourie components one obtains

$$x_k = -\frac{1}{k} J'(ek), \quad y_k = -\frac{\sqrt{1-e^2}}{ek} J'_k(ek),$$
i.e. in the considered approximation the electron moves along the closed trajectory. The forms of these expressions for $x_k$ and $y_k$ coincide with the forms of nonrelativistic ones. But in the relativistic expressions $e$ is defined by the relativistic formula (18). Let’s (following [9]) approximate Hamiltonian (16) with the Hamiltonian of pendulum with mass

$$M = |\frac{d\omega}{dn}|^{-1}$$

Then for the frequency of pendulum one has

$$\Omega = \left(\frac{ae}{2M}r_k\epsilon_k\right)^{\frac{1}{2}},$$

where $r_k = \sqrt{x_k^2 + y_k^2}$

Resonance width can be defined as in [9]

$$\Delta \nu_k = 2\Omega = 2\left(\frac{1}{2}\omega' aer_k \epsilon_k\right)^{\frac{1}{2}} = \left(2\omega' aer_k \epsilon_k\right)^{\frac{1}{2}}$$

The critical value of the external field at which chaotization of motion of the electron will occur is defined (according to [9])

$$2.5s^2 > 1,$$

where

$$s^2 = \frac{\Delta \nu_k + \nu_{k+1}}{\omega_0(k) - \omega_0(k + 1)} = \frac{(2\omega' r_k aee)^{\frac{1}{2}} + (2\omega' r_{k+1} aee)^{\frac{1}{2}}}{\omega_0(k) - \omega_0(k + 1)},$$

$$\omega_0(k) - \omega_0(k + 1) = \frac{\omega}{k} - \frac{\omega}{k + 1} = \frac{\omega}{k(k + 1)}$$

$$\Delta \nu_k = (Z\alpha)^{-\frac{5}{6}} \omega^{\frac{2}{3}} (6ee)^{\frac{1}{2}} k^{-\frac{2}{3}} r_k^{\frac{1}{2}} \left[\left(\frac{\omega}{kZ^2\alpha^2}\right)^{-\frac{2}{3}} - Z^2\alpha^2\right]^{\frac{1}{2}}$$

For the critical field we have

$$\epsilon_k = \frac{1}{\gamma_k},$$

(20)
where
\[
\gamma_k = 6(Z\alpha)^{-\frac{10}{9}}\omega^{-\frac{2}{3}}e^{\frac{2}{3}}(k+1)\{[(\frac{\omega}{kZ^2\alpha^2})^2 - Z^2\alpha^2]^\frac{1}{2}r_k^\frac{1}{2} + 
\]
\[
[(\frac{\omega}{(k+1)Z^2\alpha^2})^2 - Z^2\alpha^2]^\frac{1}{2}(1 + \frac{1}{k+1})^{-\frac{2}{3}}r_{k+1}^\frac{1}{2}\}
\]  
(21)

As is seen from this formula the critical value of the external field in the relativistic case is less than corresponding nonrelativistic case.

**Diffusive ionization**

As is well known [9], for the values of the external field strength exceeding the critical one the motion of the electron becomes chaotic and its trajectory becomes complicated and unpredicatable. This leads to the stochastic or diffusive ionization of the atom. According to [9] this process is of the diffusive character and can be described by the diffusion equation. Here we calculate coefficient of diffusion following [9] where it was done for the non-relativistic atom. From the Hamiltonian (6) one can obtain the equation for the change of the action \( n \):

\[
\frac{dn}{dt} = \frac{\partial H}{\partial \theta} = \sum F_k \cos(k\theta - \omega t),
\]

where \( F_k = \epsilon k x_k \).

Integrating this equation by the same way that was done in [9] we have

\[
(\Delta n)^2 = \pi \frac{F_k^2}{\omega_0}t
\]

From this equation we get the coefficient of diffusion

\[
D = \frac{\pi F_k^2}{2 \omega_0}
\]

Taking into account expressions for \( F_k \) and \( \omega_0 \) we have

\[
D = \frac{\pi}{2} \epsilon^2 (Z\alpha)^{-6} \omega^2 (n^2 + Z^2\alpha^2)^{\frac{9}{2}} x_k^2,
\]
where \( x_k = n\sqrt{n^2 + Z^2\alpha^2k^{-1}J'_k(\xi_k)}, \quad \omega = k\omega_0 \)

For \( k \gg 1 \) coefficient of diffusion can be written as
\[
D \approx \frac{1}{4} \epsilon^2 (Z\alpha)^4 \omega^{-\frac{3}{4}} n^2(n^2 + Z^2\alpha^2)^{\frac{1}{2}}
\]

For \( k = 1 \)
\[
D = \frac{\pi}{2} \epsilon^2 (Z\alpha)^{-2} n^2(n^2 + Z^2\alpha^2)^{\frac{5}{2}}
\]

In the general case calculation of diffusion coefficient can be performed analogously. The value of \( D \) can be obtained from (22) by the substitution
\[
x_k \longrightarrow \frac{1}{2}(x_k^2 + y_k^2)e
\]

As is seen from these formulas the coefficient of diffusion in the case of relativistic atom is greater than for the corresponding nonrelativistic one. Hence the time
\[
\tau_D \approx \frac{n^2}{2D},
\]
during which ionization of the relativistic atom will occur is less than the ionization time of the nonrelativistic atom. The ionization rate can be defined as
\[
\omega_D = \tau_D^{-1}
\]

For \( k = 1 \) we have
\[
\omega_D = \frac{1}{3}(n^2 + Z^2\alpha^2)^{5/2} = \frac{1}{3} \frac{\epsilon^2}{Z^2\alpha^2} n^5 \left(1 + \frac{5}{2} \frac{Z^2\alpha^2}{n^2} + \ldots\right),
\]
\[
\omega_{\text{nonrel}} \left(1 + \frac{5}{2} \frac{Z^2\alpha^2}{n^2} + \ldots\right), \quad (23)
\]
where
\[
\omega_{\text{nonrel}} = \frac{1}{3} \frac{\epsilon^2}{Z^2\alpha^2} n^5
\]
is the ionization rate for the nonrelativistic atom. Comparing eqs. (11) and (23) one can see that relativistic corrections to the ionization rate are considerable than relativistic corrections to the critical field.
Conclusion

We have obtained approximate analytical formula for the critical value of the field requiring for stochastic ionization of relativistic electron binding in the Coulomb field of charge \( Z \) in terms of \( Z \) and action \( n_k \). Since the relativistic Rydberg atom is an essentially quantum object, the study of its microwave field excitation, provides, therefore a testing ground for the existence of quantum relativistic ”chaotic” phenomena. More detail analysis of the above problem should be given by comparing the solution of time-dependent Dirac equation with classical equations of motion. Finally, one should note another problem which is closely related to the considered above one. Presently there is a considerable interest to the so-called chaotical autoionization of atoms and molecules [19, 20, 21]. The methods of investigations of such a systems are the same as ones for the difusive ionization [19, 20]. Therefore the above results can be also applied for the theoretical investigation of the autoionization processes of the relativistic atoms and molecules.
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