CHAOTIC AUTOIONIZATION OF RELATIVISTIC TWO-ELECTRON ATOM

D.U.MATRASULOV
Heat Physics Department of the Uzbek Academy of Sciences,
28 Katartal St.,700135 Tashkent, Uzbekistan

Abstract

Chaotic autoionization of relativistic two-electron atom in the monochromatic field is investigated. A theoretical analysis of chaotic dynamics of the relativistic outer electron under the periodic perturbation due to the inner electron, based on Chirikov criterion is given. The diffusion coefficient, the ionization rate and time are calculated.

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Study of highly excited one- and two-electron atoms on the basis of classical mechanics has been the subject of extensive theoretical [1, 2, 3] as well as experimental [4, 5] investigation recently. One of the most interesting phenomena appearing in the highly excited atom interacting with monochromatic field is the chaotization of motion of the classical electron, that leads to diffusive (or chaotic) ionization. Application of methods of stochastic dynamics to such interaction gives an important tool for these studies. In particular, the investigation of chaotization of motion of Kepler electron under the influence of monochromatic field using the Chirikov criterion allows one to estimate critical value of the field strength, at which
diffusive ionization will occur. The same type of ionization to be suggested
in the two-electron atom even in the absence of external monochromatic
field. The motion of the outer electron can become chaotic due to the inter-
action with the periodically moving inner electron that leads to the chaotic
autoionization of the outer electron. Thus the mechanism of classical au-
toionization is the following: under the influence of periodic perturbation
due to the inner electron the outer one passes to more excited orbits and
escape to infinity. Such a mechanism was first investigation by Krainov and
Belov[6]. In this Brief Report we generalize their results to the relativis-
tic case. One should note that up to now investigations of deterministic
chaos were mainly limited by the consideration of nonrelativistic systems,
though there are few works in which chaotic dynamics of relativistic sys-
tems are considered [3, 4, 11]. In our recent paper[11] we have generalized
chaotic ionization of hydrogen atom by monochromatic field to the case of
relativistic hydrogenlike atom. Further everywhere we use the relativistic
system of units \( m_e = h = c = 1 \).

Before considering the classical chaotic dynamics of the relativistic two-
electron atom we give brief classical description of the relativistic Kepler
motion in terms of action-angle variables. The Hamiltonian of the rela-
tivistic Kepler electron in the action-angle variables is [12]

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

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.

Trajectory equation of relativistic electron is given by [13]

\[
\frac{p}{r} + e \cos q \Phi - 1,
\]
where

\[ p = \frac{M^2 - Z^2\alpha^2}{EZ\alpha}, \quad q = \sqrt{1 - \frac{Z^2\alpha^2}{M^2}}, \quad e = \sqrt{1 - \frac{M^2 - Z^2\alpha^2}{n^2}}, \]  

(3)

\[ E \] is the energy of the electron.

Due to the factor \( q \) trajectory of the relativistic Kepler electron is not closed \([13]\). For 

\[ M \gg Z\alpha = \frac{Z}{137} \]  

(4)

the Hamiltonian \([11]\) takes the form

\[ H_0 = [1 + \frac{Z^2\alpha^2}{(n - M + M)^2}]^{-\frac{1}{2}} \approx \frac{n}{\sqrt{n^2 + Z^2\alpha^2}}. \]  

(5)

In this approximation \( q \approx 1 \) and trajectory becomes closed. Radius \( r \) and polar angle \( \phi \) in terms of action-angle variables can be written as

\[ r = \frac{n\sqrt{n^2 + Z^2\alpha^2}}{Z}(1 - ecos\psi), \]  

(6)

\[ ctg\phi = \frac{n}{\gamma}tg\frac{\psi}{2}, \]  

(7)

where \( \gamma = \sqrt{M^2 - Z^2\alpha^2}. \)

Consider now a relativistic two-electron atom. For the simplicity we will assume that both electrons move on the same plane. Electrons interact with the atomic core of charge \( Z\alpha. \) The Hamiltonian of two-electron atom can be written as

\[ T_1 + \frac{Z}{r_1} + T_2 - \frac{Z}{r_2} + \frac{1}{|r_1 - r_2|}, \]  

(8)

where \( T_i \) is the kinetic energies of the relativistic electrons, \( r_1 \) and \( r_2 \) are the distances from the atomic core to the inner and outer electrons, respectively; the last term in this expression describes the interelectronic repulsion. Assuming \( r_1 \ll r_2 \) the last term in (8) can be written as

\[ \frac{1}{|r_1 - r_2|} \approx \frac{1}{r_1} - \frac{r_1r_2}{r_2^3}. \]  

(9)
Inserting (9) into (8) we have

\[ T_1 + \frac{Z}{r_1} + T_2 + \frac{Z'}{r_2} + V, \tag{10} \]

where

\[ V = \frac{\mathbf{r}_1 \mathbf{r}_2}{r_2^3} \cos(\phi_1 - \phi_2), \]

\( Z' = Z - 1 \), \( \phi_1, \phi_2 \) are the azimuthal angles of the electrons on the plane of motion.

To simplify calculations we assume that the inner electron moves along the circular orbit, i.e. without eccentricity. Then from (9) we have

\[ r_1 = \frac{n_1 \sqrt{n_1^2 + Z^2 \alpha^2}}{Z} \tag{11} \]

\[ \phi = \omega_1 t = \frac{Z^2 \alpha^2}{(n_1^2 + Z^2)^{\frac{3}{4}}} \tag{12} \]

Assuming, as in [6] \( M_2/I_2 \ll 1 \), \( \cos \psi \approx 1 \), one can obtain for the outer electron

\[ r_2 = \frac{2n_2 \sqrt{n_2^2 + Z'^2 \alpha^2}}{Z'} \left( \sin^2 \psi + \frac{a^2}{4} \right), \]

where \( a = \gamma^2/n_2^2 \).

Thus perturbation can be written as

\[ V = \frac{Z'^2 \alpha^2}{4n_2^2(n_2^2 + Z'^2 \alpha^2)} r_1 (\sin^2 \psi + \frac{a^2}{4})^{-2} \cos \omega t \]

Using the Fourier expansion for the dipole moment from [6]

\[ d = (\sin^2 \psi + \frac{a^2}{4})^{-2} = \sum d_k \cos(k \theta_2), \]

where \( d_k = 26.3/(a^6 k^6) \), the full Hamiltonian can be written as

\[ H = \frac{n_2}{\sqrt{n_2^2 + Z'^2 \alpha^2}} + \epsilon \cos \omega t \sum d_k \cos(k \theta_2), \tag{13} \]

with

\[ \epsilon = \frac{Z'^2 \alpha^2}{4n_2^2(n_2^2 + Z'^2 \alpha^2)} r_1 \]
This Hamiltonian is equivalent to the one describing the interaction of relativistic hydrogenlike atom with monochromatic field \( II \) (though here \( d_k \) and \( \epsilon \) are defined by another formulae). Therefore chaotic dynamics of the outer electron can be treated by the same method as in \( II \). For the resonance width we have \( II \)

\[
\Delta \omega = 4\left(2\frac{\omega}{dn}r_1 r_2 d_k\right)^{\frac{1}{2}}
\]

(14)

The distance between two neighboring resonances is

\[
\delta \omega = \frac{\omega_1}{k^2}
\]

(15)

The Chirikov criterion for resonance overlap can be written as \( III \)

\[
2.5 \frac{\Delta \omega}{\delta \omega} > 1,
\]

This gives us (using (14) and (15))

\[
400Z^{-\frac{3}{4}}Z^{-\frac{3}{4}}n_1 n_2^5 \gamma^{-6} > 1
\]

(16)

Analogically to that as was done in \( III, IIII \) one can calculate diffusion coefficient

\[
D = \frac{\pi r_1^2 r_2^{-4} k^2 d_k^2}{2 \omega_2^2}
\]

Expressing \( r_1, r_2, d_k \) and \( \omega_2 \) via actions and charges one can obtain

\[
D \approx 68Z^6 Z^{-\frac{14}{3}}(M_2^2 - Z^2 \alpha^2)^{-6}n_1^5(n_1^2 + Z^2 \alpha^2)^{3}n_2^8(n_2^2 + Z^2 \alpha^2)^{-1}
\]

This diffusion coefficient can be written in terms of nonrelativistic one and first-order relativistic corrections as following:

\[
D \approx D_{nonrel}(1 + 3\frac{Z^2 \alpha^2}{n_1^2})(1 + 6\frac{Z^2 \alpha^2}{M_2^2})(1 - \frac{Z^2 \alpha^2}{n_2^2})
\]

(17)

where

\[
D_{nonrel} \approx 68Z^6 Z^{-\frac{14}{3}}n_1^8 n_2^6 / M_2^{12}
\]
is the nonrelativistic diffusion coefficient.

As is seen from (17) relativistic corrections to the diffusion coefficient come due to the three factors: first correction comes from increasing of the frequency of motion of the inner electron and can be considerable; second one is due to the ratio $Z\alpha/M_2$ and can be also considerable for small orbital moments; third one comes due to the relativistic motion of inner electron and leads to slight decreasing of diffusion coefficient.

Using (17) one can also calculate the ionization time [6]

$$\tau_D \approx \frac{n_2^2}{2D} \approx \tau_{\text{nonrel}}(1 - 3\frac{Z^2\alpha^2}{n_1^2})(1 - 6\frac{Z^2\alpha^2}{M_2^2})(1 + \frac{Z'^2\alpha^2}{n_2^2}).$$

Then the ionization rate per unit of time can be written as

$$\Gamma = \frac{2D}{n_2^2} \approx \Gamma_{\text{nonrel}}(1 + 3\frac{Z^2\alpha^2}{n_1^2})(1 + 6\frac{Z^2\alpha^2}{M_2^2})(1 - \frac{Z'^2\alpha^2}{n_2^2}).$$

The above formulae show that the relativistic corrections to the diffusion coefficient, autoionization time and rate are appreciable. One should note that the above results are valid for the case when $M \gg Z\alpha$. For $M > Z\alpha$ the Hamiltonian (1) becomes complex and the finite sizes of nucleus should be accounted. More detail analysis of the considered above problem should be given by solving the classical equations of motion.

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