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INTERACTION AND CHAOTIC DYNAMICS OF THE CLASSICAL HYDROGEN ATOM IN AN ELECTROMAGNETIC FIELD*

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Expressions for energy and angular momentum changes of the hydrogen atom due to interaction with the electromagnetic field during the period of the electron motion in the Coulomb field are derived. It is shown that only the energy change for the motion between two subsequent passings of the pericentre is related to the quasiclassical dipole matrix element for transitions between excited states.

1. Introduction

A classical hydrogen atom in a monochromatic electromagnetic field is one of the simplest real nonlinear systems whose dynamics may be regular or chaotic [1,2], depending on the relative field strength and frequency. Even a one-dimensional classical model of a highly excited atom yields results sufficiently close to the experimental findings. For theoretical analysis approximate mapping equations of motion, rather than differential equations, are most convenient [2-7]. Here a two-dimensional map (for the scaled energy and for relative phase of the field) is generalized for the two-dimensional hydrogen atom, i. e. we calculate energy and angular momentum changes of the atom interacting with the electromagnetic field.

2. One-dimensional atom in monochromatic field

The Hamiltonian of the hydrogen atom in a linearly polarized monochromatic electromagnetic field (in atomic units) is [4,7]

$$H = \frac{1}{2}\left(\mathbf{P} + \frac{1}{c}\mathbf{A}\right)^2 - \frac{1}{r}. \tag{1}$$

Here P is the generalized momentum, c is the light velocity,

$$\mathbf{A} = -\frac{c\mathbf{F}}{\omega}\sin(\omega t + \vartheta) \tag{2}$$

is the vector potential of the field, $\mathbf{F}$, ω, and ϑ are the field strength amplitude, field frequency, and phase, respectively. The change of the electron energy can be obtained from the Hamiltonian equations of motion [8]

$$\dot{E} = -\dot{\mathbf{r}}\mathbf{F}\cos(\omega t + \vartheta). \tag{3}$$

One can introduce the scaled energy $E_s = E/\omega^{2/3}$ and the scaled field strength $F_s = F/\omega^{4/3}$. However, it is convenient [2-7] to introduce the positive scaled energy $\varepsilon = -2E_s$ and the relative field strength $F_0 = F_s/\varepsilon_0^2$, with ε_0 being the initial scaled energy.

Integration of Eq. (3) over the period of time between two subsequent passages of the electron at the apocentre results in the change of the electron energy [3,4]

$$\varepsilon_{j+1} = \varepsilon_j - \pi F_0 \varepsilon_0^2 h(\varepsilon_{j+1})\sin\vartheta_j, \tag{4}$$

where

$$h(\varepsilon_{j+1}) = \frac{4}{\varepsilon_{j+1}} \mathrm{J}'_{s_{j+1}}(s_{j+1}). \tag{5}$$

Here $s = \varepsilon^{-3/2} = \omega/(-2E)^{3/2}$ is the relative frequency of the field, i. e. the ratio of the field frequency to the electron Kepler orbital frequency

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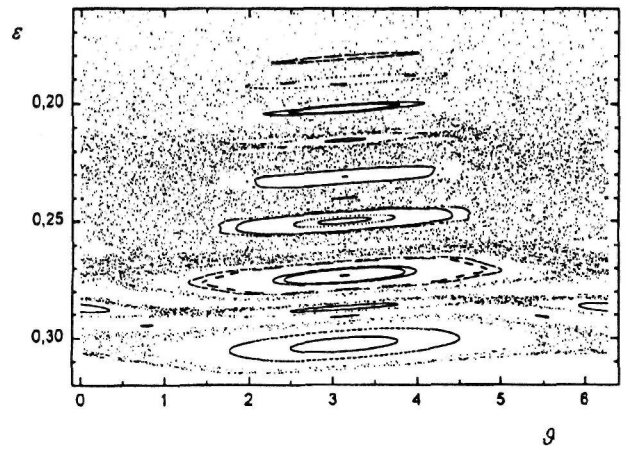

Fig. 1. Trajectories $(\mathcal{E}, \vartheta)$ for the map (4) and (6) with the parameter $\pi F_0 \mathcal{E}_0^2 = 0.0035$ and initial conditions $\vartheta_0 = \pi$, $\mathcal{E}_0 = 0.3 - 0.003i$ $(i = 0, 1, 2, \ldots)$.

and $\mathrm{J}_s'(s)$ is the derivative of the Anger function. Introducing a generating function $G(\mathcal{E}_{j+1}, \vartheta_j)$ [9, 10] one can calculate the phase ϑ change over the period

$$\vartheta_{j+1} = \vartheta_j + 2\pi\mathcal{E}_{j+1}^{-3/2} - \pi F_0 \mathcal{E}_0^2 \eta(\mathcal{E}_{j+1})\cos\vartheta_j, \qquad (6)$$

where

$$\eta(\mathcal{E}_{j+1}) = \frac{dh(\mathcal{E}_{j+1})}{d\mathcal{E}_{j+1}}. \qquad (7)$$

Equations (4) and (6) describe the changes of the energy and phase in time. This map greatly facilitates numerical investigation of dynamics and ionization processes. In Figs. 1 and 2 results of the numerical analysis of the map (4) and (6) are presented.

3. Two-dimensional atom in monochromatic field

For calculation of the energy change of the arbitrarily oriented two-dimensional atom in the electromagnetic field according to Eq. (3), one should perform the transformation of the coordinates (Fig. 3). The change of the angular momentum of the atom follows from the Hamiltonian equations of motion

$$\dot{M} = -\frac{\partial H}{\partial \alpha} = -rF\sin(\alpha + \varphi)\cos(\omega t + \vartheta). \qquad (8)$$

By analogy with the scaled energy one can introduce the scaled angular momentum $\mu = 2M_s = 2M\omega^{1/3}$. Moreover, it is convenient to introduce the parametric equations of motion for

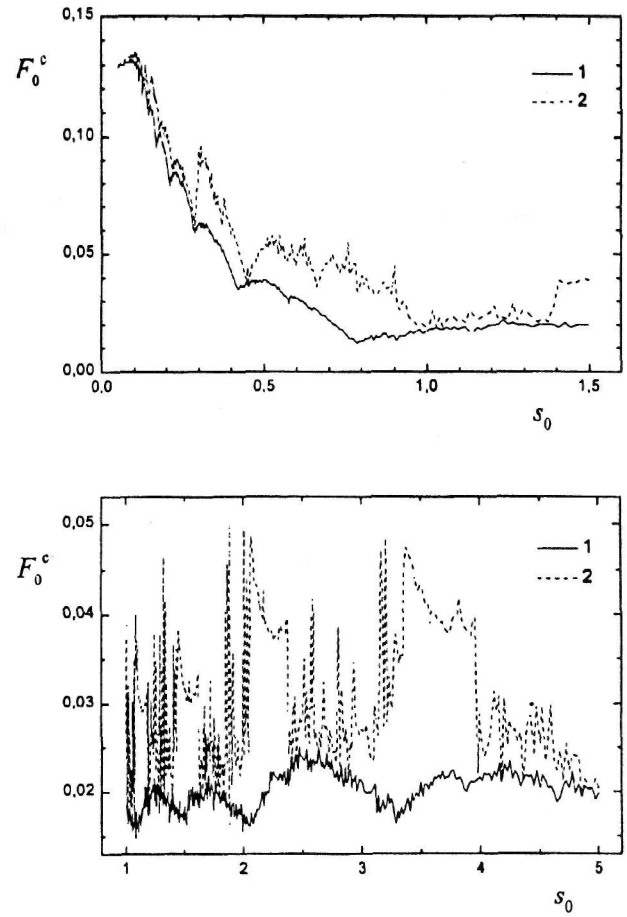

Fig. 2. The ionization threshold field dependence on the relative frequency s_0. Continuous curve represents results calculated with variation of the initial phase ϑ_0, while dotted curve is for $\vartheta_0 = 0$.

the Coulomb potential [6-8].

Integration of Eqs. (3) and (8) for half of the period of the electron motion, i. e. for transition from apocentre to pericentre, yield the scaled energy and angular momentum changes in the linearly polarized electromagnetic field

$$\mathcal{E}_{j+1} = \mathcal{E}_j + \frac{2\pi F_0 \mathcal{E}_0^2}{\mathcal{E}_{j+1}} \times$$

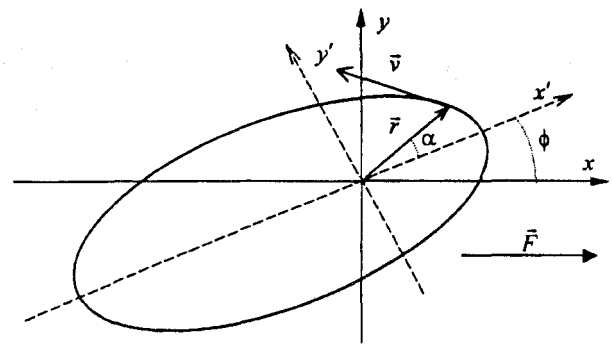

Fig. 3. Two-dimensional atom in the electromagnetic field.

$$\times \left\{ -\left[\mathrm{J}_s'(z)\sin\vartheta_j + \mathrm{E}_s'(z)\cos\vartheta_j \right]\cos\varphi + \frac{\sqrt{1-e^2}}{e}\left[\left(\mathrm{J}_s(z) - \frac{\sin(s\pi)}{s\pi} \right)\cos\vartheta_j - \left(\mathrm{E}_s(z) - \frac{1-\cos(s\pi)}{s\pi} \right)\sin\vartheta_j \right]\sin\varphi \right\} \quad (9)$$

and

$$\mu_{j+1} = \mu_j + \frac{2\pi F_0 \mathcal{E}_0^2}{\mathcal{E}_{j+1}} \left\{ \frac{\sqrt{1-e^2}}{e}\left[\left(\mathrm{J}_s(z) - \frac{\sin(s\pi)}{s\pi} \right)\sin\vartheta_j + \left(\mathrm{E}_s(z) - \frac{1-\cos(s\pi)}{s\pi} \right)\cos\vartheta_j \right]\cos\varphi \right.$$

$$\left. + \left[\left(-\mathrm{J}_s'(z) + (1+e)\frac{\sin(s\pi)}{\pi} \right)\cos\vartheta_j + \left(\mathrm{E}_s'(z) + (1+e)\frac{\cos(s\pi)}{\pi} + \frac{1-e}{\pi} \right)\sin\vartheta_j \right]\sin\varphi \right\}. \quad (10)$$

Here $\mathbf{E}_s(z)$ is the Weber function, $z = es$ and e is the eccentricity of the ellipsis. By analogy or from Eqs. (9) and (10) choosing appropriate initial phases of the field one can calculate the energy and angular momentum changes for the electron motion from pericentre to apocentre as well as for the complete period with different initial conditions.

So, for motion between two subsequent passages at the apocentre we have generalization of Eq. (4) for the energy change

$$\mathcal{E}_{j+1} = \mathcal{E}_j + \frac{4\pi F_0 \mathcal{E}_0^2}{\mathcal{E}_{j+1}} \left\{ -\mathrm{J}_s'(z)\sin\vartheta_j\cos\varphi + \frac{\sqrt{1-e^2}}{e}\left[\mathrm{J}_s(z) - \frac{\sin(s\pi)}{s\pi} \right]\cos\vartheta_j\sin\varphi \right\} \quad (11)$$

and the angular momentum change

$$\mu_{j+1} = \mu_j + \frac{4\pi F_0 \mathcal{E}_0^2}{\mathcal{E}_{j+1}} \left\{ \frac{\sqrt{1-e^2}}{e}\left[\mathrm{J}_s(z) - \frac{\sin(s\pi)}{s\pi} \right]\sin\vartheta_j\cos\varphi + \left[-\mathrm{J}_s'(z) + (1+e)\frac{\sin(s\pi)}{\pi} \right]\cos\vartheta_j\sin\varphi \right\}. \quad (12)$$

One can calculate the energy and angular momentum changes for the electron motion between two subsequent passages at the pericentre in a similar way.

3.1. Approximation for relatively high frequency s

For relatively high frequency of the field $s \gg 1$, the asymptotic form of the Anger function $\mathbf{J}_s(se)$ and its derivative $\mathbf{J}_s'(se)$ may be used [7]. Then Eq. (11) may be written in the form

$$\mathcal{E}_{j+1} = \mathcal{E}_j + \pi F_0 \mathcal{E}_0^2 \left\{ (e-2)\left[4b - \frac{4a}{5}\mathcal{E}_{j+1} - \frac{\sin(\mathcal{E}_{j+1}^{-3/2}\pi)}{\pi}\mathcal{E}_{j+1}^2 \right]\sin\vartheta_j\cos\varphi + \frac{\sqrt{1-e^2}}{e}\left[4a\mathcal{E}_{j+1}^{-1/2} \right.\right.$$

$$\left.\left. - \frac{2\sin(\mathcal{E}_{j+1}^{-3/2}\pi)}{\pi}\mathcal{E}_{j+1}^{1/2} - \frac{2b}{35}\mathcal{E}_{j+1}^{3/2} + (e-1)\left(4b\mathcal{E}_{j+1}^{-3/2} - \frac{4a}{5}\mathcal{E}_{j+1}^{-1/2} - \frac{\sin(\mathcal{E}_{j+1}^{-3/2}\pi)}{\pi}\mathcal{E}_{j+1}^{1/2} \right) \right]\cos\vartheta_j\sin\varphi \right\}. \quad (13)$$

Introducing the generating function we can obtain the iterative equation for the phase ϑ_j as a generalization of Eq. (6)

$$\vartheta_{j+1} = \vartheta_j + 2\pi\mathcal{E}_{j+1}^{-3/2} + \pi F_0 \mathcal{E}_0^2 \left\{ (2-e)\left[\frac{4a}{5} - \frac{3\cos(\mathcal{E}_{j+1}^{-3/2}\pi)}{2}\mathcal{E}_{j+1}^{-1/2} + \frac{2\sin(\mathcal{E}_{j+1}^{-3/2}\pi)}{\pi}\mathcal{E}_{j+1} \right]\cos\vartheta_j\cos\varphi + \frac{\sqrt{1-e^2}}{e} \times \right.$$

$$\left. \times \left[2a\mathcal{E}_{j+1}^{-3/2} - 3\cos(\mathcal{E}_{j+1}^{-3/2}\pi)\mathcal{E}_{j+1}^{-2} + \frac{\sin(\mathcal{E}_{j+1}^{-3/2}\pi)}{\pi}\mathcal{E}_{j+1}^{-1/2} + \frac{3b}{35}\mathcal{E}_{j+1}^{1/2} + (e-1)\left(6b\mathcal{E}_{j+1}^{-5/2} - 2a\mathcal{E}_{j+1}^{-3/2} \right.\right.\right.$$

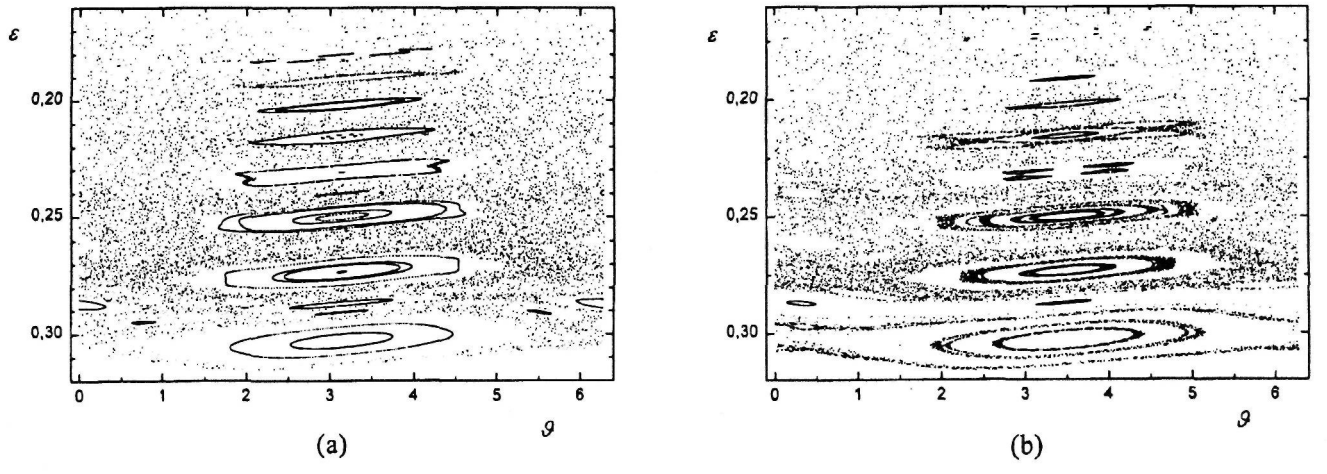

Fig. 4. Phase plane $(\mathcal{E}, \vartheta)$ of the two-dimensional map (13) and (14) with parameter $\pi F_0 \mathcal{E}_0^2 = 0.0035$, initial conditions $\vartheta_0 = \pi$, $\mathcal{E}_0 = 0.3 - 0.003i$ $(i = 0, 1, 2, \ldots)$ and orientation angle (a) $\varphi = 0$ and *(b)* $\varphi = \pi/6$.

$$-\frac{3\cos(\mathcal{E}_{j+1}^{-3/2}\pi)}{2}\mathcal{E}_{j+1}^{-2} + \frac{\sin(\mathcal{E}_{j+1}^{-3/2}\pi)}{2\pi}\mathcal{E}_{j+1}^{-1/2}\Bigg)\Bigg]\sin\vartheta_j\sin\varphi\Bigg\}. \tag{14}$$

Using mapping Eqs. (13) and (14) we can represent the energy and phase dynamics (Fig. 4) and calculate numerically the relative threshold field strength for the ionization of the two-dimensional hydrogen atom (Fig. 5).

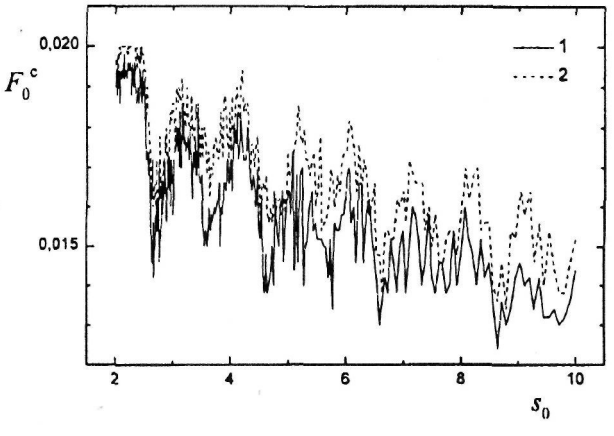

Fig. 5. The ionization threshold field dependence on the relative frequency s_0 for a two-dimensional atom with the eccentricity $e = 0.9$ and orientation angle $\varphi = 0$ (curve *1)* and $\varphi = \pi/6$ (curve 2).

3.2. Limiting cases for energy and angular momentum changes

3.2.1. Approximations for very extended orbits

For very extended orbits, $e \to 1$, the expansions for the energy (11) and angular momentum (12) in powers of $\beta = \sqrt{1 - e^2} \ll 1$ are

$$\mathcal{E}_{j+1} = \mathcal{E}_j + \frac{4\pi F_0 \mathcal{E}_0^2}{\mathcal{E}_{j+1}}\left\{-(1+\beta^2)\mathrm{J}_s'(s)\sin\vartheta_j\cos\varphi + \beta\left[\mathrm{J}_s(s) - \frac{\sin(s\pi)}{s\pi}\right]\cos\vartheta_j\sin\varphi\right\}, \tag{15}$$

$$\mu_{j+1} = \mu_j + \frac{4\pi F_0 \mathcal{E}_0^2}{\mathcal{E}_{j+1}}\left\{\beta\left[\mathrm{J}_s(s) - \frac{\sin(s\pi)}{s\pi}\right]\sin\vartheta_j\cos\varphi + \left[-(1+\beta^2)\mathrm{J}_s'(s) + (2-\beta^2)\frac{\sin(s\pi)}{\pi}\right]\cos\vartheta_j\sin\varphi\right\}. \tag{16}$$

For $e = 1$ Eq. (15) coincides with Eq. (4) for the one-dimensional atom, while Eq. (16) represents change of the angular momentum resulting in the transition to the elliptic states with nonzero angular momentum.

3.2.2. Approximations for almost circular orbits

For almost circular orbits the eccentricity is small, $e \to 0$. Expansion of expressions (11) and (12) in powers of e may be obtained from Eqs. (3) and (11). The results are

$$\varepsilon_{j+1} = \varepsilon_j + \frac{4F_0\varepsilon_0^2\sin(s\pi)}{\varepsilon_{j+1}}\left\{\left[\frac{e}{2} + \frac{\frac{3}{4}e^2s^2 - 1}{1-s^2} + \frac{\frac{1}{2}es^2}{4-s^2} - \frac{\frac{3}{4}e^2s^2}{9-s^2}\right]\sin\vartheta_j\cos\varphi\right.$$

$$\left. + s\left[\frac{1-\frac{1}{4}e^2\left(s^2-4\right)}{1-s^2} - \frac{e}{4-s^2} + \frac{\frac{1}{4}e^2s^2}{9-s^2}\right]\cos\vartheta_j\sin\varphi\right\}, \tag{17}$$

$$\mu_{j+1} = \mu_j + \frac{4F_0\varepsilon_0^2\sin(s\pi)}{\varepsilon_{j+1}}\left\{s\left[-\frac{e}{2} + \frac{1-e^2\left(1+\frac{1}{4}s^2\right)}{1-s^2} + \frac{e\left(1-\frac{1}{2}s^2\right)}{4-s^2} - \frac{\frac{1}{4}e^2s^2}{9-s^2}\right]\sin\vartheta_j\cos\varphi\right.$$

$$\left. + \left[\frac{3e}{2} + \frac{s^2\left(\frac{1}{2}e^2\left(1+\frac{1}{2}s^2\right)-1\right)}{1-s^2} - \frac{\frac{1}{2}es^2}{4-s^2} + \frac{\frac{1}{2}e^2s^2\left(3-\frac{1}{2}s^2\right)}{9-s^2}\right]\cos\vartheta_j\sin\varphi\right\}. \tag{18}$$

These expansions are not valid for $s = 1,2,3,\ldots$.

4. Atom in the circularly polarized field

The equation for the energy change of the atom in the circularly polarized field is

$$\dot{E}_k = -eF\left[v_x\cos(\omega t + \vartheta) \pm v_y\sin(\omega t + \vartheta)\right]. \tag{19}$$

Here sign '+' or '-' corresponds to the same and opposite directions of the electron and field rotations, respectively.

For the electron moving between two subsequent pericentres the energy and angular momentum changes are

$$\varepsilon_{j+1} = \varepsilon_j - \frac{4\pi F_0\varepsilon_0^2}{\varepsilon_{j+1}}\left\{J'_{-s}(z) \pm \frac{\sqrt{1-e^2}}{e}\left[J_{-s}(z) - \frac{\sin(s\pi)}{s\pi}\right]\right\}\sin(s\pi + \vartheta_j \mp \varphi), \tag{20}$$

$$\mu_{j+1} = \mu_j + \frac{4\pi F_0\varepsilon_0^2}{\varepsilon_{j+1}}\left\{\left[\frac{\sqrt{1-e^2}}{e}\left(J_{-s}(z) - \frac{\sin(s\pi)}{s\pi}\right) \mp \left(-J'_{-s}(z) + (e-1)\frac{\sin(s\pi)}{\pi}\right)\right]\sin(s\pi + \vartheta_j \mp \varphi)\right.$$

$$\left. \pm \frac{(1+1/e)\cos(s\pi) + 1 - 1/e}{\pi}\cos(s\pi + \vartheta_j \mp \varphi)\right\}. \tag{21}$$

It should be noted that expression in the curly brackets in Eq. (20) coincides with the expression of the quasiclassical radial dipole matrix element in the velocity representation [6]

$$D_p^{\pm} = \frac{1}{s}\left\{J'_{-s}(z) \pm \frac{\sqrt{1-e^2}}{e}\left[J_{-s}(z) - \frac{\sin(s\pi)}{s\pi}\right]\right\}. \tag{22}$$

This correspondence, however, takes place only for interaction of the hydrogen atom with the circularly polarized microwave field and for integration of the equations of motion between two subsequent pericentres. In general, the energy [3,7] and angular momentum changes depend on the integration interval. So, for motion of the electron between two subsequent apocentres, i. e. the points most distant from the nucleus, where the electron's energy change is minimal, the energy change is described by the expression similar to Eq. (20) but instead of $J_{-s}(es)$ and $J'_{-s}(es)$ we have the Anger function and its derivative of the positive order, $J_s(es)$ and $J'_s(es)$. This interval has been used in Refs. [3-5] for derivation of the Kepler map for the one-dimensional hydrogen atom.

5. Conclusion

Analytical expressions for the energy and angular momentum changes of the two-dimensional hydrogen atom in linearly and circularly polarized electromagnetic fields are derived. It should be noted that in general the expressions are rather

complicated. The approximate expressions for limiting cases of the parameters are more convenient for analytical and numerical analysis of the dynamics.

The derived expressions are suitable for the three-dimensional hydrogen atom as well and may be generalized for analysis of the chaotic motion (due to the Jupiter perturbations) of comets and asteroids in the Sun system.

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