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Research paper

To and fro motion for the hydrogen atom in a circularly polarized microwave field

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ABSTRACT

We study the problem of the hydrogen atom interacting with a circularly polarized microwave field, and more specifically, we focus on the so called to and fro motion, that is, the erratic trajectories described by the electron making several large distance excursions and close passages to the nucleus. The skeleton of such trajectories is based on the so called ejection-collision orbits (ECO), that is, orbits ejected from the nucleus, describing several far/close passages to the origin and finally colliding with it. The computation and continuation of families of ECO, as well as their bifurcations is analysed, and finally the consequences of such orbits to explain to and from motion as well as ionization of an electron by the external field are also described.

1. Introduction

The study of the n-body problem, and in particular, the 3-body problem in Celestial Mechanics has been the keystone to advance in the understanding of different aspects of classical mechanics –both from a physical and mathematical point of view–. Chaotic dynamics is an intriguing one. However, chaos appears also in the microscopic or quantum problems. It is remarkable how the study of the Restricted three body problem –which may be regarded as a perturbation of the Kepler problem–, is a paradigm problem in the macroscale mechanics and a vast literature has been, and still is, devoted to it (see [3,5,6,16] and references therein). In the microscale or quantum mechanics, there exists an analogue problem which is the hydrogen atom interaction with a circularly polarized electromagnetic field, called from now on the CP problem. This problem, in rotating coordinates becomes a Keplerian problem plus a perturbation depending on one parameter and the equations of motion for the electron can be written as a Hamiltonian system of ordinary differential equations (ODE) which has a unique singularity that corresponds to the collision with the nucleus (located at the origin). Thus, the tools from a dynamical system approach that are applied for the RTBP may be used in the CP problem.

Many references have been devoted to this problem (see for example [1,2,4,12] and references therein); the last one being the first systematic study of the relevant invariant objects in phase space which control the dynamics, but more focused on ionizing/escaping orbits. However none of them analyse a mechanism that explains the naive behaviour of the so called to and fro motion, that is, the behaviour of the electron when it describes a trajectory with several far and close passages to the nucleus in an erratic or chaotic way. An approach to this mechanism is studied in [1]; nevertheless, in that paper,

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the authors considered different sets of initial conditions and integrated numerically the CP system of ODE but stopped the numerical integration when the electron was close to the nucleus due to the presence of the singularity. Therefore no results about the behavior of trajectories passing very close of the origin were given. In the present paper, we regularize the equations of motion to remove the singularity, so this difficulty is completely overcome. More precisely, we study orbits that eject from (or collide with) the origin and have several close passages to it. The skeleton of the to and fro motion consists of what we call n ejection-collision orbits (denoted from now on as n-ECO). An n-ECO is a trajectory that ejects from the nucleus (origin), has $2n-1$ extrema in the distance to the origin (typically corresponding to n maxima and $n-1$ minima), and collides with the nucleus. We will show how these ECO are simply heteroclinic connections between different equilibrium points and we study their existence when varying the energy. This approach was originally applied in the RTBP, and partial analytical results are obtained in [8–10] for the circular RTBP and in [11,15] for the elliptic case. A massive numerical analysis for the circular RTBP is recently carried out in [14]. Finally we will discuss the role that such ECO play on the global dynamics of the CP problem, concerning not only the to and fro motion, but the non-return (or ionization) as well.

The paper is organized as follows: in Section 2 we provide the system of ordinary differential equations (ODE) governing the motion for the electron in a rotating system of coordinates. Some basic and known properties of this problem, concerning equilibrium points, periodic orbits and possible regions of motion, are shortly recalled. In Section 3 we explain the methodology to deal with ECO: the regularization of the singularity at the origin of the system of ODE is carried out, the collision manifold is studied (which provides an insight about how orbits passing close to the collision will behave) and the strategies to compute ECO and the organization of ECO in families (and bifurcations) are described. The convenience to use suitable Poincaré sections is also discussed. Section 4 is devoted to provide and describe the results obtained from massive simulations. The possibility of having ejection orbits that finally ionize is also explained taking into account the values of the energy of the CP problem. Fynally, some conclusions are drawn in Section 5.

We finally remark that the numerical integrations of the systems of ODE done along the paper use a Taylor method implemented on a robust, fast and accurate software package by Jorba and Zou ([7]).

2. Description of the CP problem. Main features

In order to have a self contained paper, we present the main features of this problem. The details can be found in [1].

We consider the relative motion of a hydrogen atom submitted to a circularly polarized (CP) microwave, where the pulse of the microwave field is taken with a *flat-top* shape, that is, the field amplitude is ramped up in time until it achieves a final, constant amplitude. In this study we ignore the ramping and just consider the dynamics after the flat-top has been reached (see[2] for a discussion of the consequences of the initial ramp).

The Hamiltonian for the electron of the hydrogen atom (in the limit of an infinitely massive nucleus and in atomic units $m_e = \hbar = e = 1$) subjected to a CP microwave field is the following:

$$\tilde{H}(X, Y, X', Y', Z, Z') = \frac{1}{2}(X'^2 + Y'^2 + Z'^2) - \frac{1}{R} + F(X\cos\omega s + Y\sin\omega s), \tag{1}$$

where (X, Y, Z) are the position coordinates, $R^2 = X^2 + Y^2 + Z^2$, s is the time, $' = \frac{d}{ds}$, ω is the angular frequency of the microwave field and $F > 0$ is the field strength (see[2]). We will consider the motion in the planar case, that is for $Z = 0$. Furthermore, we take a rotating frame with the CP field, that is, (x, y) coordinates such that

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \cos\omega s & -\sin\omega s \\ \sin\omega s & \cos\omega s \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Defining now the momenta $p_x = \dot{x} - \omega y$ and $p_y = \dot{y} + \omega x$, the transformed Hamiltonian becomes

$$\hat{H}(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) - \omega(xp_y - yp_x) - \frac{1}{R} + Fx,$$

being $R = \sqrt{x^2 + y^2}$.

Now we simplify this Hamiltonian re-scaling time and distances. We define a new time $t = \omega s$ and consider the symplectic change of coordinates with multiplier $\omega^{-1/3}$, more precisely,

$$(x, y) = \omega^{-2/3}(\bar{x}, \bar{y}), \qquad (p_x, p_y) = \omega^{1/3}(\bar{p}_x, \bar{p}_y).$$

The transformed Hamiltonian becomes in the new variables (for simplicity, we drop the bar and we keep the same names for the position and momentum coordinates),

$$H(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) - xp_y + yp_x - \frac{1}{r} + Kx, \tag{2}$$

where $K = F/\omega^{4/3} > 0$ and now $r = \sqrt{x^2 + y^2}$, $p_x = \frac{dx}{dt} - y$ and $p_y = \frac{dy}{dt} + x$.

A first remark is that we obtain an autonomous Hamiltonian, depending on the parameter $K > 0$, with two degrees of freedom, which turns out to be a perturbation of the well known Kepler problem. So for K very small, we should expect the typical dynamics of a Hamiltonian system close to an integrable one, but of course with the features of a non integrable one.