Physica D 241 (2012) 333-349

Contents lists available at SciVerse ScienceDirect

Physica D



journal homepage: www.elsevier.com/locate/physd

Phase space structure of the hydrogen atom in a circularly polarized microwave field

Esther Barrabés^{a,*}, Mercè Ollé^b, Florentino Borondo^c, David Farrelly^d, Josep M. Mondelo^e

^a Dept. Informàtica i Matemàtica Aplicada, Universitat de Girona, 17071 Girona, Spain

^b Dept. de Matemàtica Aplicada I, Universitat Politècnica de Catalunya, Barcelona, Spain

^c Departamento de Química, and Instituto Mixto de Ciencias Matemáticas CSIC–UAM–UC3M-UCM, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain

^d Department of Chemistry and Biochemistry, Utah State University, Logan, UT 84322-0300, United States

^e IEEC & Dept. Matemàtiques, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

ARTICLE INFO

Article history: Received 15 June 2011 Received in revised form 30 September 2011 Accepted 3 October 2011 Available online 12 November 2011 Communicated by K. Josic

Keywords: Hamiltonian dynamical systems Perturbed problem Periodic orbits Chaotic regions Ionization

1. Introduction

ABSTRACT

We consider the problem of the hydrogen atom interacting with a circularly polarized microwave field, modeled as a perturbed Kepler problem. A remarkable feature of this system is that the electron can follow what we term erratic orbits before ionizing. In an erratic orbit the electron makes multiple large distance excursions from the nucleus with each excursion being followed by a close approach to the nucleus, where the interaction is large. Here we are interested in the mechanisms that explain this observation. We find that the manifolds associated with certain hyperbolic periodic orbits may play an important role, despite the fact that, in some respects, the dynamics is almost Keplerian. A study of some relevant invariant objects is carried out for different system parameters. The consequences of our findings for ionization of an electron by the external field are also discussed.

© 2011 Elsevier B.V. All rights reserved.

Studies of the three body problem and, in particular, the Sun-Earth-Moon system, have stimulated an enormous number of advances in physics and mathematics, including the discovery of classical chaos [1]. Obviously chaotic dynamics, e.g., in the Solar System, can have a variety of consequences many of which might be considered negative or destructive. However, recently chaos has been implicated in the construction of various objects in the Solar System, e.g., binaries in the Kuiper belt as well as the capture of irregular moons at Jupiter and Saturn [2]. Chaos is far from being a topic restricted to classical mechanics; over the past forty years or so a vast body of literature has accumulated on the subject of chaos in microscopic, i.e., quantum, systems. Many of these studies have focused on perturbations of the hydrogen atom which is described by the same (classical) Hamiltonian as is Kepler's problem. We mention in particular [3-6], (going back 10-15 years) to the latest application [7] (and also references therein) corresponding to strong field ionization.

* Corresponding author. *E-mail address:* barrabes@ima.udg.edu (E. Barrabés).

In classical mechanics, Hill's problem, which is essentially a perturbed Kepler problem, is widely viewed as being the paradigm of a realistic chaotic system (although other simple models certainly exist). Hill's problem can be obtained as a special case of the restricted three-body problem (RTBP). It is of note that in quantum mechanics a very close analogue to the RTBP exists, namely, the hydrogen atom interaction with a circularly polarized electromagnetic fields-which we will refer here simply as "the CP" problem (see, for example, [8,9]). All of the ingredients of the RTBP are contained in this system; stable or unstable motion in a rotating frame depending on a parameter; the possibility of capture or escape (of an electron); stable, unstable and chaotic motion co-existing well above all equilibrium points of the system. The latter point is significant because escape and capture are not governed by energy constraints, i.e., by surfaces of zero-velocity, but by dynamical constraints which are not immediately obvious based on a study of the potential energy surface or the surface of zero-velocity. In the CP problem these properties have been used to predict and simulate electronic states which are direct analogs of the Trojan asteroids in the Solar System; essentially these states are highly localized electronic wavepackets which "orbit" the nucleus in much the same way that the two groups of Trojan asteroids orbit the Sun along the same orbit as does Jupiter [10,11].

