Computational Investigation of the Interaction Between Hydrogen Atoms and an Intense Circularly Polarized Laser Field

Lifeng Yang^{1,2}, Wang Xu^{1,*}, Qiren Zhang³, Wen Luo^{1,2}, Qiangyan Pan¹, Xiaolu Cai^{1,2}, Gongtao Fan^{1,2}, Yongjiang Li^{1,2}, Benji Xu¹, Zhe Yan¹, Guangwei Fan^{1,2} and Zhendong An^{1,2}

 ¹ Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China.
² Graduate School of the Chinese Academy of Sciences, Beijing 10039, China.

³ Departments of Technical Physics, Peking University, Beijing 100871, China.

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Abstract. The study of interactions between a high-power laser and atoms has been one of the fundamental and interesting topics in strong field physics for decades. Based on a nonperturbative model, ten years ago, we developed a set of programs to facilitate the study of interactions between a circularly polarized laser and atomic hydrogen. These programs included only contribution from the bound states of the hydrogen atom. However, as the laser intensity increases, contribution from continuum states to the excitation and ionization processes becomes larger and can no longer be neglected. Furthermore, because the original code is not able to add this contribution directly due to its many disadvantages, a major upgrade of the code is required before including the contribution from continuum states in future. In this paper, first we deduce some important formulas for contribution of continuum states and present modifications and tests for the upgraded code in detail. Second we show some comparisons among new results, old results from the original codes and the available experimental data. Overall the new result agrees with experimental data well. Last we present our calculation of above-threshold ionization (ATI) rate and compare it with a pertubative calculation. The comparison shows that our nonperturbative calculation can also produce ATI peak suppression.

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*Corresponding author. *Email address:* xuwang@sinap.ac.cn (W. Xu)

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1 Introduction

The study of interaction between a strong laser field and atoms originated from the perturbation theoretical study for two-photon transition by Göeppert-Mayer [1] in 1931. However, the first experimental observation of atomic multiphoton ionization (MPI) [2,3] only took place in late 1960 after the laser was invented [4]. In early experiments, laser intensity $(I < 10^{12} \text{W/cm}^2)$ was much lower than atomic coulomb field (10^{16}W/cm^2) . Therefore, the MPI could be accurately described by Low Order Perturbation Theory (LOPT) [5–7]. However, LOPT has difficulties in explaining some nonperturbative phenomena such as near-resonant MPI [8], and AC Stark shift of atomic energy levels [9], which occurs when the laser intensity was sufficiently high. Although the perturbation theory included higher order perturbation extensions to explain these phenomena, it has already become necessary to study these phenomena under nonperturbative framework. In fact, the nonperturbative era for the study of interaction between a strong laser field and atoms did not truly begin until Above Threshold Ionization (ATI), a nonperturbative phenomenon, was discovered by P. Agostini from studying the interaction between a laser field and atomic silver [10] in 1979. Since then, many other new nonperturbative phenomena such as High Harmonic Generation (HHG) [11–14] and Stabilization [15–18] were discovered. In the past two years, due to the breakthrough of high-power and longwave laser techniques [19], Low-Energy Structures (LES) [20, 21], another novel nonperturbative phenomenon, was discovered. In addition, the study of atomic behavior in a field of the ultra-short super intense laser [22–24] recently became possible because of the development of ultra-short free electron lasers (FELs) in the extreme ultraviolet (XUV) to hard-*x*-ray wavelength regime [25,26]. More new nonperturbative phenomena are therefore expected to be observed in the near future. Because of all these, we foresee the study the interactions between high-power lasers and atoms to continue for decades.

Due to the simplicity of the hydrogen atom, there have been some experimental studies on the interaction of an intense laser with hydrogen atoms [27–31]. Although linearly polarized lasers, rather than circularly polarized lasers, are typically used in these experiments, the theoretical study of the interactions between circularly polarized lasers and hydrogen atoms is a basic topic and an important component in strong field physics. The earliest of such studies using nonperturbative theory is from the Keldysh-Faisal-Reiss (KFR) type theories based on strong field approximation in 1980s [32]. In the late 1980s, the Floquet theory was used in those studies [33–35]. In recent years, some theoretical physicists have directly solved two-dimension (2D) and three-dimension (3D) cases of the time-dependent Schrodinger equation (TDSE) of hydrogen atoms in an intense circularly polarized laser field [36–39]. We have focused on this study for more than a decade as well. Based on non-relativistic and dipole approximation, we built a nonperturbative model for solving the TDSE of hydrogen atom in a circularly polarized laser field [40,41]. Using this model and the Jacobi algorithm, we developed a FORTRAN program (Q1) with quadruple precision to facilitate this study. Later on, we upgraded Q1 to another FORTRAN program (Q2) by replacing the Jacobi algorithm with the Givens algorithm