Optics Communications 313 (2014) 74–79

Contents lists available at ScienceDirect

Optics Communications

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

Multiphoton and tunneling ionization probability of atoms and molecules in an intense laser field

Song-Feng Zhao *, Lu Liu, Xiao-Xin Zhou *

College of Physics and Electronic Engineering, Northwest Normal University, Key Laboratory of Atomic and Molecular Physics and Functional Materials of Gansu Province, Lanzhou 730070, China

ARTICLE INFO

Article history:
Received 12 July 2013
Received in revised form
23 September 2013
Accepted 25 September 2013
Available online 19 October 2013

Keywords:
Multiphoton ionization
Tunneling ionization
Tunneling ionization models
Time-dependent Schrödinger equation

ABSTRACT

We theoretically studied ionization of atoms exposed to an intense laser field by using three different methods, i.e., the numerical solution of the single-active-electron approximation based time-dependent Schrödinger equation (SAE-TDSE), the Perelomov–Popov–Terent'ev (PPT) model, and the Ammosov–Delone–Krainov (ADK) model. The ionization of several linear molecules in a strong laser field is also investigated with the molecular ADK (MO-ADK) and the molecular PPT (MO-PPT) model. We show that the ionization probability from the PPT and the MO-PPT model agrees well with the corresponding SAE-TDSE result in both the multiphoton and tunneling ionization regimes. By considering the volume effect of the laser field, the ionization signal obtained from the PPT and the MO-PPT model fits well the experimental data in the whole range of the multiphoton and tunneling ionization regimes. However, both the ADK and MO-ADK models seriously underestimate the ionization probabilities (or signals) in the multiphoton regime.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

Ionization of atoms and molecules is the first step of many interesting strong-field phenomena such as high-order harmonic generation (HHG), high-energy above-threshold ionization (HATI) and molecular imaging by the recolliding electrons [1–3]. Multiphoton ionization of atoms in a weak laser field was widely studied both experimentally and theoretically after the discovery of lasers [4,5]. It was found that an atom exposed to a high-frequency and low-intensity laser field can be ionized by simultaneously absorbing several photons (the so-called multiphoton ionization), which is firstly observed by Voronov and Delone [6]. The valence electron in an atom can also be removed by tunneling through the potential barrier formed by the Coulomb force and the strong laser field, i.e., tunneling ionization [7–11]. The pioneering theoretical works on the ionization of atoms in a laser field were achieved based on the Keldysh theory [12]. According to the Keldysh theory, different ionization mechanisms of atoms and molecules can be distinguished by the Kelydsh parameter $\gamma = \sqrt{I_p/2U_p} = \omega\sqrt{2I_p}/F$, where I_p is the ionization potential of atoms and molecules, ω is the laser angular frequency, F is the electric field strength and U_p is the ponderomotive energy. It is known that tunneling ionization dominates if $\gamma < 1$, while multiphoton ionization will prevail when $\gamma > 1$. These days the accurate ionization probability of atoms can be easily obtained by solving the single-active-electron approximation based time-dependent Schrödinger equation (SAE-TDSE) [13–15]. The exact static ionization rates of the He atom have also been calculated by solving the full two-electron TDSE in which the electron–electron correlation effects have been included [16]. The multiphoton ionization probability of He, Ne and Ar was determined using the time-dependent density functional theory (TDDFT) where the multielectron correlation has been partially considered [17].

In addition to these elaborate calculations, some simpler models were proposed to calculate the ionization rate of atoms, such as the Keldysh–Faisal–Reiss (KFR) theory [12,18,19], the Ammosov–Delone–Krainov (ADK) model [20], the Perelomov–Popov–Terent'ev (PPT) model [21–23], and so on. The ADK model has been confirmed to fit well the TDSE results and the experimental data in the tunneling ionization regime [14–16,24]. However, it found that the ADK model overestimates the ionization rate of atoms in the over-the-barrier ionization (OBI) regime [14–16]. Tong and Lin [15] proposed an improved ADK (so-called TBI) model to calculate the ionization rate of atoms in the OBI regime. The validity of the TBI model has been carefully examined by comparing with the TDSE calculations. In our previous work [25], we found that the ADK model fails to give the correct ionization probability in the multiphoton ionization regime, while the PPT model agrees well with those SAE-TDSE calculations in both the

* Corresponding authors. Tel.: +86 9317971148.
E-mail addresses: zhaosf@nwnu.edu.cn (S.-F. Zhao), zhouxx@nwnu.edu.cn (X.-X. Zhou).

0030-4018/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.optcom.2013.09.074

multiphoton and tunneling ionization regimes. On the experimental side, the PPT and the ADK model were used to fit the experimental ionization signals of several rare gas atoms using a 200 fs Ti-sapphire laser pulse with the central wavelength of 800 nm [11]. They found that the PPT model excellently fits all the experimental data covering a quite wide range from multiphoton to tunneling ionization regimes, while the ADK model fits only in the range where $\gamma < 0.5$.

Tunneling ionization of molecules in the presence of a low-frequency strong laser field has been widely studied [26,27], especially for the orientation-dependent ionization rate [28–35] and the ionization suppression of molecules compared to their companion atoms [36–44]. This is because the orientation-dependent ionization rate (or probability) P(θ) of a molecule fixed in space can be used to directly image the electronic structures of the ionizing orbitals from which the active electron is removed, where θ is the angle between the molecular axis and the laser's polarization direction. Theoretically P(θ) can be obtained by solving the TDSE mostly based on the SAE approximation [33,45–48]. The multielectron effect of P(θ) can be considered within the framework of the TDDFT [34,49–51]. Since both these two methods are rather time-consuming to obtain P(θ), many simpler theoretical models are proposed, such as the molecular strong-field approximation (MO-SFA) theory [44,52] and the molecular tunneling ionization (MO-ADK) model [43,53–57]. The MO-ADK model has also been empirically modified to study the ionization of the H_2^+ molecule in the OBI regime [15]. The another molecular tunneling ionization (MO-PPT) model [41] was used to successfully predict the ionization suppression of Cl_2 in comparison to Xe. Recently the weak-field asymptotic theory (WFAT) based on the stationary Schrödinger equation of molecules in a static electric field was developed to study the tunneling ionization of molecules [58–61].For molecules, whether the MO-PPT and the MO-ADK model can fit the SAE-TDSE calculations and the experimental data or not?

The main goal of this paper is to carefully examine the PPT and the MO-PPT model by comparing ionization probabilities (or signals) with those of the accurate SAE-TDSE calculations and the experimental data. The rest of this paper is arranged as follows. In Section 2, we describe how to calculate ionization probabilities of atoms by solving the TDSE with the generalized pseudospectral method [62,63]. The basic equations of the ADK, the PPT, the MO-ADK and the MO-PPT model are briefly reviewed. In Section 3, we study the laser wavelength dependence of ionization probabilities of the H atom with the PPT model and compare them with those of the SAE-TDSE. Then we show how the PPT and the MO-PPT model fit the TDSE results and the experimental data in the whole range of multiphoton and tunneling ionization regimes. The large deviations of the ADK and MO-ADK models with respect to the SAE-TDSE method and the experimental results are also presented. A conclusion is given in Section 4. Atomic units are used throughout this paper unless otherwise stated.

2. Theoretical methods

The theory part is separated into three subsections. First, we describe how to obtain the accurate ionization probabilities of atoms by solving the SAE-TDSE. We then briefly review the basic equations of the ADK, the PPT, the MO-ADK and the MO-PPT model. Finally, we present how to calculate the ionization probability and signal of atoms and molecules once the static ionization rate is obtained.

2.1. TDSE method of atoms

Using the SAE approximation and the length gauge, the TDSE of atoms in the presence of a linearly polarized laser field can be written as

$$i\frac{\partial}{\partial t}\psi(\mathbf{r},t) = [H_0(\mathbf{r}) + H_i(\mathbf{r},t)]\psi(\mathbf{r},t) \tag{1}$$

where $H_0(\mathbf{r})$ is the field-free Hamiltonian

$$H_0(\mathbf{r}) = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{L^2}{2r^2} + V(\mathbf{r}) \tag{2}$$

The atomic model potential $V(\mathbf{r})$ is parameterized as [15]

$$V(r) = -\frac{1 + a_1 e^{-a_2 r} + a_3 r e^{-a_4 r} + a_5 e^{-a_6 r}}{r} \tag{3}$$

For the He, Ne and Ar targets, all the parameters in Eq. (3) can be found in Ref. [15]. For the Xe atom, a_1, a_2, a_3, a_4, a_5 and a_6 are taken to be 51.3555, 2.1116, −99.9275, 3.7372, 1.6445 and 0.4306, respectively. For the Kr atom, we use the model potential proposed by Garvey et al. [64].

The electron–field interaction $H_i(\mathbf{r},t)$ can be expressed as

$$H_i(\mathbf{r},t) = -zF(t) \tag{4}$$

Eq. (1) can be efficiently solved by using the time-dependent generalized pseudospectral method [62,63]. In the present calculations, we use the following absorbing function:

$$\cos^{0.25}[\pi(r - r_0)/2(r_{max} - r_0)] \tag{5}$$

for $r \geq r_0$ and 1.0 elsewhere. Once the time-dependent wavefunction is obtained, the total ionization probability of atoms at the end of laser field can be calculated by

$$P_{tot} = 1 - \langle \psi(\mathbf{r}, t_{final}) | \psi(\mathbf{r}, t_{final}) \rangle \tag{6}$$

2.2. The ADK and the PPT model

According to the ADK model [20], the static tunneling ionization rate is given by

$$w_{ADK}(F) = |C_{n^*l^*}|^2 f(l,m) E_0 \left(\frac{2F_0}{F}\right)^{2n^* - |m| - 1} \exp\left(-\frac{2F_0}{3F}\right) \tag{7}$$

In the PPT model [21–24], the ionization rate in a static field can be written as

$$w_{PPT}(F,\omega) = |C_{n^*l^*}|^2 f(l,m) E_0 \left(\frac{2F_0}{F}\right)^{2n^* - |m| - 1} (1+\gamma^2)^{|m|/2 + 3/4} A_m(\omega,\gamma) \times \exp\left(-\frac{2F_0}{3F} g(\gamma)\right) \tag{8}$$

where

$$|C_{n^*l^*}|^2 = \frac{2^{2n^*}}{n^* \Gamma(n^* + l^* + 1)\Gamma(n^* - l^*)} \tag{9}$$

$$f(l,m) = \frac{(2l+1)(l+|m|)!}{2^{|m|}(|m|)!(l-|m|)!} \tag{10}$$

$$g(\gamma) = \frac{3}{2\gamma}\left[\left(1 + \frac{1}{2\gamma^2}\right)\sinh^{-1}\gamma - \frac{\sqrt{1+\gamma^2}}{2\gamma}\right] \tag{11}$$

where $F_0 = (2E_0)^{3/2}$ and $n^* = Z_c(2E_0)^{-1/2}$. Here E_0 and Z_c are the binding energy and the asymptotic charge, respectively. l and m are the orbital and magnetic quantum numbers of the active electron of the atom, respectively. The effective orbital quantum number $l^* = n^* - 1$ and the coefficients $A_m(\omega,\gamma)$ can be found in Refs. [21,24,25].

2.3. The MO-ADK and the MO-PPT model

We assume that the molecular axis is aligned along the external field direction. In the MO-ADK model [43,55,57], the tunneling

Download English Version:

https://daneshyari.com/en/article/1534786

Download Persian Version:

https://daneshyari.com/article/1534786

Daneshyari.com