Multiphoton and tunneling ionization of atoms in an intense laser field*

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We study the ionization probabilities of atoms by a short laser pulse with three different theoretical methods, i.e., the numerical solution of the time-dependent Schrödinger equation (TDSE), the Perelomov–Popov–Terent'ev (PPT) theory, and the Ammosov–Delone–Krainov (ADK) theory. Our results show that laser intensity dependent ionization probabilities of several atoms (i.e., H, He, and Ne) obtained from the PPT theory accord quite well with the TDSE results both in the multiphoton and tunneling ionization regimes, while the ADK results fit well to the TDSE data only in the tunneling ionization regime. Our calculations also show that laser intensity dependent ionization probabilities of a H atom at three different laser wavelengths of 600 nm, 800 nm, and 1200 nm obtained from the PPT theory are also in good agreement with those from the TDSE, while the ADK theory fails to give the wavelength dependence of ionization probability. Only when the laser wavelength is long enough, will the results of ADK be close to those of TDSE.

Keywords: intense laser field, ionization probability, multiphoton ionization theory

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1. Introduction

With the rapid development of laser techniques in the past decades, strong-field phenomena such as high-order harmonic generation (HHG), high-energy above-threshold ionization (HATI), and multiple ionization have been investigated experimentally and theoretically.[1−5] Since ionization of atoms is the first step to all these rescattering processes, much attention has been paid to studies on the ionization of atoms in an intense laser field.[2,6]

It is known that an atom can be ionized through different mechanisms, which are distinguished by Keldysh parameter[7] $\gamma = \sqrt{I_{\rm p}/2U_{\rm p}} = \omega\sqrt{2I_{\rm p}}/F$, where$I_{\rm p}$ is the ionization potential of atoms, $U_{\rm p}$ is the ponderomotive energy, ω is the laser angular frequency, and F is the electric field strength. Note that tunneling ionization will dominate if $\gamma < 1$, while multiphoton ionization prevails when $\gamma > 1$. Theoretically, the accurate ionization probability of atoms can be obtained by solving the time-dependent Schrödinger equation (TDSE) mostly based on the single-active-electron (SAE) approximation.[8] Since the TDSE has to be solved hundreds of times when macroscopic effects of HHG are considered,[9] such calculations are rather time-consuming. Thus some simpler models are quite desirable. The Keldysh–Faisal–Reiss (KFR) theory[7,10,11] is used to treat the tunneling ionization of atoms in a strong laser field, which has been extended to the case of molecules (the so-called MO-SFA).[12,13] The Ammosov-Delone-Krainov (ADK) theory[14] is another alternative model used to study the tunneling ionization of atoms, which is also generalized to molecular systems (i.e., MO-ADK theory).[15−17] Tong and Lin[18] have further extended the ADK theory to the near- or over-the-barrier ionization regime by modifying the original ADK theory with an empirical correction factor. The ADK theory has been confirmed by comparing it with the TDSE calculations and experimental data in the tunneling ionization regime.[18−20] In order to calculate ionization probabilities more efficiently for the numerical solution of the Maxwell equation when the macroscopic propagation of HHG is taken into account, Gaarde

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et al.[9] have proposed obtaining the accurate tunneling ionization probability of an argon atom with the ADK theory multiplied by a laser intensity dependent correction factor which can be determined by fitting the ADK results to those of the TDSE. Only when $\gamma < 0.5$,[21] is the ADK theory proved to fit well to the experimental ionization signals for several rare gas atoms (i.e., He, Ne, Ar, Kr, and Xe). Otherwise, the remarkable discrepancies between the ADK and the experimental results occur. Another tunneling ionization model proposed by Perelomov, Popov and Terent'ev (PPT)[22−24] is found to fit quite well to the experimental ionization signals in the multiphoton and tunneling ionization regimes. It is of importance to carefully examine the PPT theory with the more accurate TDSE calculations. So far there has been no direct comparison between the calculations from the TDSE and those from the PPT.

The main goal of this paper is to compare the ionization probabilities of atoms obtained from the PPT theory with those TDSE results from multiphoton to tunneling ionization regimes, and the validity of ADK is also checked in the multiphoton ionization regime. On the other hand, the laser wavelength dependence of ionization probabilities of atoms is also investigated with the TDSE, the PPT and the ADK, respectively. The rest of this paper is arranged as follows. In Section 2, we describe how to calculate ionization probabilities of atoms by the TDSE, the PPT and the ADK. The basic equations of these three methods are also briefly reviewed. In Section 3, we compare ionization probabilities of atoms by a short laser pulse obtained from the TDSE, the PPT and the ADK. A conclusion is given in Section 4. Atomic units are used throughout this paper unless otherwise stated.

2. Theoretical method

The theory part is separated into two subsections, in which we will describe how to calculate the ionization probabilities of atoms in a short laser pulse by solving the TDSE and by using the PPT and the ADK theories.

2.1. TDSE method

Based on the SAE approximation, the TDSE of atoms exposed to a linearly polarized laser field in the length gauge can be expressed as

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

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

$$H_0(\boldsymbol{r}) = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{L^2}{2r^2} + V(\boldsymbol{r}). \tag{2}$$

The atomic model potential $V(\boldsymbol{r})$ is parameterized as[18]

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

The parameters in Eq. (3) for the targets used in this paper can be found in Ref. [18].

The electron-field interaction $H_{\mathrm{i}}(\boldsymbol{r},t)$ can be written as

$$H_{\mathrm{i}}(\boldsymbol{r},t) = -zF(t). \tag{4}$$

Equation (1) can be efficiently solved by a time-dependent generalized pseudospectral method.[25,26] In order to avoid the reflection of the wavefunction at the boundary, the absorbing function takes the form $\cos^{0.25}[\pi(r-r_0)/2(r_{\max}-r_0)]$ for $r \geq r_0$.

Once the time-dependent wavefunction is available, the ionization probability of atoms at the end of laser field can be determined by

$$P = 1 - \langle\psi(\boldsymbol{r},t_{\mathrm{final}})|\psi(\boldsymbol{r},t_{\mathrm{final}})\rangle. \tag{5}$$

2.2. PPT theory and ADK theory

Based on the PPT theory, the ionization rate in a static field is given by[19,22]

$$\begin{aligned} w_{\mathrm{PPT}}(F,\omega) = {} & |C_{n^*l^*}|^2 f(l,m) E_0 \left(\frac{2F_0}{F}\right)^{2n^*-|m|-1} \\ & \times (1+\gamma^2)^{|m|/2+3/4} \\ & \times A_m(\omega,\gamma)\exp\left(-\frac{2F_0}{3F}g(\gamma)\right), \end{aligned} \tag{6}$$

where

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

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

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

$$\begin{aligned} A_m(\omega,\gamma) = {} & \frac{4}{\sqrt{3\pi}}\frac{1}{|m|!}\frac{\gamma^2}{1+\gamma^2} \\ & \times \sum_{\kappa\geq\nu}^{\infty}\mathrm{e}^{-\alpha(\gamma)(\kappa-\nu)} w_m(\sqrt{\beta(\gamma)(\kappa-\nu)}), \end{aligned}$$

$$w_m(x) = \frac{x^{2|m|+1}}{2}\int_0^1 \frac{\mathrm{e}^{-x^2 t}t^{|m|}}{\sqrt{1-t}}\,\mathrm{d}t,$$

$$\alpha(\gamma) = 2\left(\sinh^{-1}\gamma - \frac{\gamma}{\sqrt{1+\gamma^2}}\right),$$
$$\beta(\gamma) = \frac{2\gamma}{\sqrt{1+\gamma^2}},$$
$$\nu = \frac{E_0}{\omega}\left(1 + \frac{1}{2\gamma^2}\right),$$
$$\kappa = \left\langle \frac{E_0}{\omega} + 1 \right\rangle + S, \quad (S = 0, 1, \ldots).$$

The symbol $\langle\ \rangle$ indicates the integer part of the value inside. Here $F_0 = (2E_0)^{3/2}$ with E_0 being the electron binding energy, the effective principal quantum number $n^* = Z_c\,(2E_0)^{-1/2}$ with Z_c being the asymptotic charge and the effective orbital quantum number $l^* = n^* - 1$.

According to the ADK theory,[14,18] the static field tunneling ionization rate can be expressed as

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

Once the static field ionization rates for a given atom are available, we can calculate the total ionization probability by a laser pulse as

$$P = 1 - \exp\left(-\int_{-\infty}^{+\infty} w_m\left[|F(t)|\right] \mathrm{d}\,t\right), \quad (8)$$

where m stands for PPT or ADK.

3. Results and discussion

Typically the truncated radii $r_{\max} = 400$ a.u. and $r_0 = 350$ a.u. the total number of grid points $N = 800$, and up to 60 partial waves are used in the TDSE simulations. The electric field is taken to be in the form of

$$F(t) = F_{\rm p} \mathrm{e}^{-2\ln 2t^2/\tau^2} \cos(\omega t + \varphi), \quad (9)$$

where $F_{\rm p}$ is the electric field peak strength and τ is the full width at half maximum (FWHM) of the laser pulse. $\tau = 10$ fs is used in this paper and the carrier-envelope phase (CEP) φ is only taken to be 0. We check that the pulse duration and CEP have little effect on the ionization probability of atoms.

Figure 1 shows the ionization probabilities versus peak intensity for three different targets (i.e., H, He, and Ne). Note that ionization probabilities calculated from the PPT theory and the ADK theory are normalized to those of the TDSE at the saturation laser intensity for a given atom. The laser wavelength $\lambda = 800$ nm is used for H atom, and $\lambda = 400$ nm for He and Ne. To more easily distinguish between the multiphoton and tunneling ionization regions, the values of Keldysh parameter γ are also labeled on the top of each panel. In Fig. 1, we can see the ionization probabilities from the PPT accord quite well with those of the TDSE in the range from multiphoton to tunneling ionization, while the ADK results fit well to the ionization probabilities obtained from the TDSE only in the range where $\gamma < 1$. In the multiphoton ionization region, the discrepancies between the ADK and the TDSE become larger as the laser intensity decreases. The largest deviation of the ADK with respect to the TDSE reaches three orders of magnitude for He atom and five orders of magnitude for H atom and Ne atom.

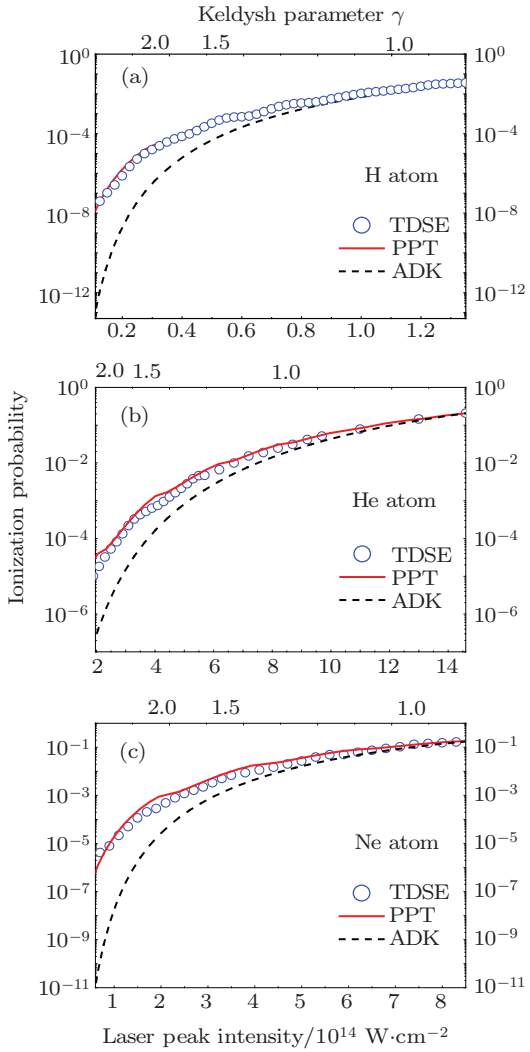


Fig. 1. (colour online) Comparisons of ionization probabilities of atoms versus laser peak intensity, obtained from the TDSE, the PPT and the ADK: (a) is for H atom at laser wavelength $\lambda = 800$ nm, (b) is for He atom at $\lambda = 400$ nm, (c) is for Ne atom at $\lambda = 400$ nm.

In addition, the ionization probabilities of atoms depend on the parameters of the laser pulse. It is of interest to study the effect of laser wavelength on the ionization probability of atoms. In Fig. 2 we show the laser intensity dependent ionization probabilities of a H atom at three different laser wavelengths. For simplicity, all the ionization probabilities presented in Fig. 2 are normalized to be 1.0 at the saturation intensity. In Fig. 2, we can see that the ionization probabilities obtained from the TDSE and the PPT depend on the laser wavelength, while those from the ADK do not depend on the laser wavelength as expected in Eq. (7). For the PPT theory, the wavelength dependence of ionization probability can be attributed to the functions $A_m(\omega,\gamma)$, $(1+\gamma^2)^{|m|/2+3/4}$ and $g(\gamma)$ in Eq. (6). The ionization probabilities obtained from the TDSE and the PPT at three different laser wavelengths are found to be in good agreement in Fig. 2. The ionization probability monotonically increases as the laser wavelength decreases, with the laser intensity fixed. That means the deviation of the ADK from the TDSE becomes larger with laser wavelength decreasing. In other words, the ADK results should be close to those from the TDSE only when the laser wavelength is long enough. Therefore the wavelength dependence of ionization probability in the case of lower laser intensity is stronger than in the case of the higher intensity. We find that the ionization probabilities from the ADK tend to equal those obtained from the PPT due to $A_m(\omega,\gamma)\to 1$, $\left(1+\gamma^2\right)^{|m|/2+3/4}\to 1$ and $g(\gamma)\to 1$ in the tunneling ionization region ($\gamma << 1$) (see Eqs. (6) and (7)).

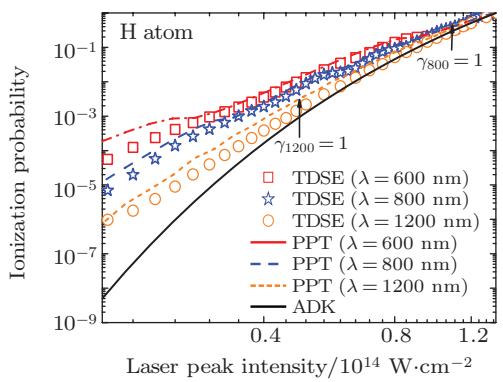


Fig. 2. (colour online) Comparisons of normalized ionization probabilities of hydrogen atom versus laser intensity at three different laser wavelengths ($\lambda=600$ nm, 800 nm, and 1200 nm).

4. Conclusion

In this paper we compare ionization probabilities by a short laser pulse of atoms, obtained from the PPT theory and the ADK theory with those obtained from the TDSE method. We find that the ionization probabilities from the PPT accord quite well with those from the TDSE in a wider range from multiphoton to tunneling ionization, while the ADK results are reliable only in the tunneling ionization regime as expected. We also demonstrate that the PPT theory can well predict the wavelength dependence of ionization probability of a H atom compared with the TDSE, while the ADK fails to give the wavelength dependence of the ionization probability. Since the TDSE calculations are rather time-consuming when the macroscopic propagation of HHG is theoretically considered, out of the fact that the PPT theory can fit well to the TDSE results presented in this paper and also to the experimental data in Ref. [21], we suggest that the ionization rate or the ionization probability is calculated directly using the PPT theory rather than the numerical solution of the TDSE equation.

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