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Ionization suppression of diatomic molecules in different wavelength laser fields

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ABSTRACT

We theoretically study ionization of the N_2 and O_2 molecules and focus on the ionization suppression at various wavelengths. We find that the ionization rate of the N_2 molecules is not significantly suppressed over a wide range of laser wavelengths. The ratio of the ion yields of N_2^+ to that of Ar^+, however, slightly decreases as the laser wavelength increases, and this ratio for the low laser intensity is slightly larger than that for the high laser intensity. The interference effect greatly modulates the photoelectron energy spectra: an interference valley appearing in the photoelectron energy spectra. For the O_2 molecules, the ionization suppression is always significant, and clearly depends on the laser wavelength and the laser intensity. The ratio of the ion yields of O_2^+ to that of Xe^+ becomes larger as the laser wavelength (intensity) increases under given laser intensity (wavelength). Overall photoelectron energy spectra of O_2 are suppressed, especially for the low-energy range.

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1. Introduction

The ionization of atoms and molecules in strong laser pulses is an important strong field process. Compared with atoms whose ionization dynamics in a strong laser field are essentially determined by their binding energies and the laser parameters, molecules have additional parameters to be considered, such as the orbital symmetry, orientation of the molecules with respect to the laser field polarization, which may also have strong influences on the photoionization dynamics [1–5]. The *ionization suppression* is one of the most fundamental differences between a molecule and the atom with similar binding energy. Earlier studies indicated that the total ionization rates of some diatomic molecules in intense laser fields are nearly equal to those of reference atoms with similar binding energy [6–8], while recent studies show that this is not always true [9]. For example, the ionization rate of N_2 molecule remains comparable to that of Ar atom, while the ionization rate of O_2 molecule is lower than that of Xe atom by more than one order of magnitude. Motivated by these experimental and theoretical findings, many studies for the ionization suppression have been performed [5,10–12]. When we turn to the ionization suppression of diatomic molecules, however, there are only a few studies on the dependence of ionization suppression on the laser wavelength. In recent studies, Durá et al. [13] and Lin et al. [14] experimentally and theoretically investigated the ionization suppression of molecules in strong laser field with different laser wavelengths. They found that the ionization rate of N_2 molecule is almost identical to that of Ar atom, irrespective of laser wavelength. In contrast, the ionization rate of O_2 molecule is distinctively suppressed compared to Xe atom, and the suppression is more obvious at laser wavelength of 0.8 μm. In Ref. [13], Durá et al. had discussed the wavelength dependence of the suppressed ionization of N_2 and O_2 at laser intensity of 10^{14} W/cm^2, and in Ref. [14], Lin et al. had discussed the suppressed ionization of N_2 and O_2 at two special laser wavelengths of 0.8 μm and 2.0 μm.

In order to show the ionization suppression of N_2 and O_2 in the different wavelength laser fields and at the different laser intensities, and to get deep insight into the ionization suppression, in this paper, we follow the treatment in Ref. [15] to investigate the wavelength-dependence of ionization suppression of O_2 and N_2 molecules under different laser intensities. We perform comprehensive calculations on the ionization rates and the photoelectron energy spectra by a linearly polarized laser field.

This paper is arranged as follows: we introduce the ionization rate formula used in this paper in Section 2, and the results and discussions are in Section 3. In Section 4, we conclude.

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2. Ionization-rate formula

In the theoretical study on the photoionization processes of atoms and molecules in intense laser fields, the strong-field approximation is widely used [17–19]. In this approximation, the Coulomb attraction of the parent ion to the ionized electron is neglected. In order to treat the influence of the Coulomb attraction, a correction is made on the continuum state of the electron in the laser field [16]. Within this correction, the ionization-rate formula of photoelectrons with a fixed kinetic energy in strong laser field is given by [16,19–21] (the units $c=\hbar=1$ are used throughout this paper)

$$\frac{dW}{d\Omega_{\mathbf{P}_f}}=\frac{m_e\omega^2}{(2\pi)^2}\sum_{n=n_0}^{N}(n-u_p)^2|\mathbf{P}_f| \times|\mathcal{X}_n(Z,\eta)|^2|\Phi(\mathbf{P}_f,\mathbf{R})|^2, \quad (1)$$

where $d\Omega_{\mathbf{P}_f}=\sin\theta_f\,d\theta_f\,d\phi_f$ is the differential solid angle of the momentum of photoelectron $\mathbf{P}_f$, θ_f and ϕ_f are its emission and azimuthal angles, respectively; $\varepsilon_b=E_b/\omega$ is the molecular binding energy in the unit of laser-photon energy ω, n is the number of the photon absorbed, and $n_0=[u_p+\varepsilon_b]_{int}+1$ is the minimum number of photon absorbed during ionization; $u_p=U_p/\omega$ is the ponderomotive parameter of the laser fields defined as

$$u_p=\frac{e^2I}{2m_e\omega^3}$$

with I being the laser intensity. In Eq. (1), we use a generalized phased Bessel (GPB) function, which was introduced in Ref. [22] and used in the following papers [23–26]. By means of the phased Bessel function $X_n(Z)$ which relates to the ordinary Bessel function as

$$X_n(Z)=J_n(r)e^{in\varphi},\quad Z=re^{i\varphi},$$

the GPB function is defined as

$$\mathcal{X}_n(Z,\eta)=\sum_{k=-\infty}^{+\infty}X_{n-2k}(Z)X_k(\eta). \quad (2)$$

The two arguments in Eq. (2) are defined as follows:

$$Z=\frac{e\sqrt{2I}}{m_e\omega^2}\boldsymbol{\varepsilon}\cdot\mathbf{P}_f,\quad \eta=-\frac{1}{2}u_p\cos\xi, \quad (3)$$

where $\boldsymbol{\varepsilon}$ is the polarization vector of the laser field, and ξ denotes the degree of the polarization, such that $\xi=0$ and $\pi/2$ correspond to the linear and the circular polarization, respectively.

In Eq. (1), $\Phi(\mathbf{P}_f,\mathbf{R})$ is the molecular wave function in momentum space which reads

$$\Phi(\mathbf{P}_f,\mathbf{R})=\int d\mathbf{r}\exp(-i\mathbf{P}_f\cdot\mathbf{r})\Phi(\mathbf{r},\mathbf{R}), \quad (4)$$

where $\Phi(\mathbf{r},\mathbf{R})$ is the initial wave function of O_2 and N_2 molecules and $R\equiv|\mathbf{R}|$ is the internuclear distance. According to the linear combination of atomic shell theory [16,27], the initial wave function of O_2 and N_2 molecules has the following form:

$$\Phi(\mathbf{r},\mathbf{R})=\frac{\Phi_i(\mathbf{r}+\mathbf{R}/2)\pm\Phi_i(\mathbf{r}-\mathbf{R}/2)}{\sqrt{2(1\pm S(R))}}, \quad (5)$$

where $\Phi_i(\mathbf{r})$ are the initial atomic wave function of the valence electron. The minus sign on the right-hand side corresponds to an antibonding valence orbital ($1\pi_g$ for O_2), whereas the plus sign corresponds to a bonding valence orbital ($3\sigma_g$ for N_2). The atomic orbital overlap integral $S(R)$ is defined as

$$S(R)=\int d\mathbf{r}\Phi_i(\mathbf{r}+\mathbf{R}/2)\Phi_i(\mathbf{r}-\mathbf{R}/2)^*, \quad (6)$$

which varies with the internuclear distance $R\equiv|\mathbf{R}|$. The Fourier transform of $\Phi(\mathbf{r},\mathbf{R})$, i.e., the wave function in momentum space, is worked out to be analytically [16]

$$\Phi_{O_2}(\mathbf{P}_f,\mathbf{R})=\frac{\mathcal{C}(\kappa)2^6p_f(\pi a^7)^{1/2}}{(a^2+p_f^2)^3}\frac{\sin(\mathbf{P}_f\cdot\mathbf{R}/2)\sin(\varphi_p)}{\sqrt{2(1-S(R))}},$$
$$\Phi_{N_2}(\mathbf{P}_f,\mathbf{R})=\frac{\mathcal{C}(\kappa)2^6p_f(\pi a^7)^{1/2}}{(a^2+p_f^2)^3}\frac{\cos(\mathbf{P}_f\cdot\mathbf{R}/2)\cos(\varphi_p)}{\sqrt{2(1+S(R))}}, \quad (7)$$

where φ_p is the polar angle of photoelectron momentum with respect to the molecular axis, $a=\alpha 2E_b$ is the Bohr radius and α is the fine structure constant, and $p_f=|\mathbf{P}_f|$. The quantity $\mathcal{C}(\kappa)=(2\kappa E_b/E)^{\kappa^{-1}}$ is the Coulomb correction factor, and $\kappa=1/a$, and E is the peak field strength of the incident laser.

3. Numerical results and discussion

In our calculations, the wavelength of laser field varies from 0.8 μm to 2.0 μm and the laser fields are linearly polarized. The laser intensity varies from 5×10^{13} to 10^{14} W/cm^2. As for the molecules, we have supposed that the molecular axis $\mathbf{R}$ is in the xy plane, that is, $\theta_m=\pi/2$. According to Eq. (1), we calculate the ionization rates of molecules and atoms from the photoelectrons

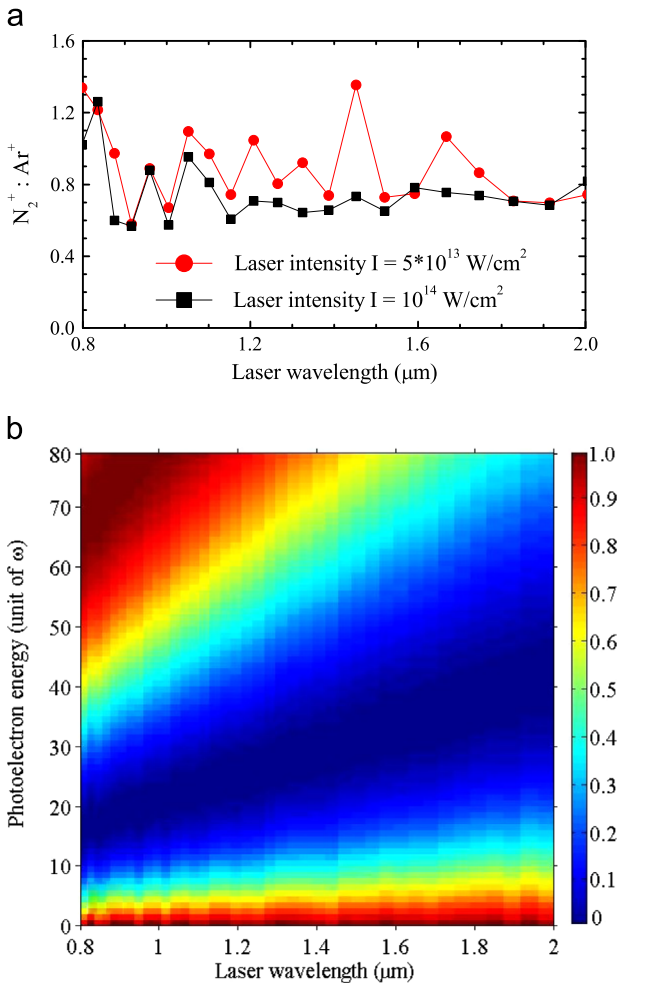

Fig. 1. (a) Ratio of the ion yields of N_2^+ to that of Ar^+ as a function of the laser wavelength under two laser intensities. Molecules are assumed to be randomly oriented in the xy plane. (b) Value of the interference factor, $|\cos(P_fR/2)|$, as functions of laser wavelength and photoelectron energy. The molecular axis is supposed to be along the laser polarization vector.

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