Calculation of the photoelectron spectra under a scaling transform*

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(Received 30 March 2012; revised manuscript received 6 August 2012)

By solving the time-dependent Schrödinger equation, the dependence of photoelectron energy spectra on the binding energy of targets, wavelength and the intensity of laser pulse is exhibited and a scaling law of kinetic energy spectra of both the direct and the rescattered photoelectrons is concluded. The scaling law provides a convenient tool to determine the equivalent photoionization process of various atoms or molecules in various laser fields. The verification of the scaling law by independent methods provides incontestable support to the validity of the scaling law.

Keywords: scaling law, photoelectron energy spectrum, rescattering process

PACS: 32.80.Rm, 42.65.Ky, 12.20.Ds, 03.65.Nk **DOI:** 10.1088/1674-1056/22/1/013207

1. Introduction

Above-threshold ionization[1] (ATI) and the accompanying high-order harmonic generation[2] (HHG) are two fundamental processes where atoms and molecules are irradiated by intense laser fields, in which scaling analysis provides a new insight into various phenomena.[3] Many papers have contributed to the scaling law of ATI and HHG. For example, in order to increase the harmonic yields and to obtain attosecond pulses, many authors studied the scaling relationship of high-order harmonic generation on the wavelength of the driving laser fields. Various scaling relationships were established.[4–7] Most scaling relationships focus on the dependence of HHG yields on the wavelength but the necessary physical insight is not enough, while very few scaling relationships were established and discussed for ATI.

The outgoing electrons from ATI carry information of atomic structures, thus studies on ATI enrich our knowledge of the atomic structures as well as the physical process itself. A generally accepted picture of ATI is as follows: under the action of an intense laser field, the bound electrons in atoms are excited then they move in the laser field. If the electrons leave the laser field immediately, they generally obtain less kinetic energy and are called as directly emitted photoelectrons. If the electrons do not leave the laser field before the electric field of the laser pulse inverses, they will be driven back to then be rescattered by their parent core and thus obtain a larger kinetic energy. This fraction of electrons called the rescattered photoelectrons has been used to retrieve accurate information of atomic cores.[8–10]

For directly emitted photoelectrons, our analytical study is based on the nonperturbative quantum electrodynamic theory of ATI[11,12] has disclosed a scaling law of photoelectron angular distributions (PADs).[13] The scaling law indicates that the main characteristics of PADs are determined by three dimensionless parameters: 1) the ponderomotive number $u_p = U_p/\omega$, i.e., the ponderomotive energy U_p in units of photon energy ω; 2) the binding number $\varepsilon_b = E_b/\omega$, i.e., the binding energy of the atomic target in the unit of ω; 3) the number of absorbed photons during ionization. When these three parameters are unchanged, the main features of PADs are the same. The scaling law enables us to obtain the identical PADs as well as physical processes when the frequency of the driving laser fields changes. Subsequent studies show that the scaling law holds for both directly emitted and rescattered photoelectrons[14] in both long-pulsed[13] and few-cycle laser fields.[15]

The scaling law of rescattered photoelectrons is of great importance, since the scaling law provides a necessary reference that can be used to classify different experimental results, by which the structure of targets is retrieved. Using the recently derived analytical formulae,[16] we find that, under the scaling transform, both the kinetic energy spectra and the PADs of rescattered photoelectrons remain unchanged. The scaling law indicates that the physical essence of interaction processes with the same parameters are just the same, even though their dynamic parameters look quite different. Recently, in a study using the rescattered photoelectrons to retrieve the core information of target atoms,[8–10] as well as the tomography of the outmost shell of target molecules by HHG,[17] a reference is needed that can be obtained by the

*Project supported by the National Natural Science Foundation of China (Grant Nos. 61078080 and 11174304) and the National Basic Research Program of China (Grant Nos. 2010CB923203 and 2011CB808103).

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scaling law.

Verifications by independent methods provide a strong check to the scaling law. The scaling law of rescattered photoelectrons is established by an analytical formula and is verified by the numerical results based on the formula. Independent verifications come from two sources, one is the experimental observations and the other is the theoretical verification by means of different methods, such as the numerical study based on the time-dependent Schrödinger equation (TDSE) method.

In this paper, we perform a detailed study on the kinetic energy spectra of photoelectrons from atoms irradiated by laser fields of various wavelengths and different intensities, by means of the numerical solution of the three-dimensional TDSE. We will show that the photoelectron energy spectra vary notably with the binding energy of target atoms and the frequency and the intensity of driving laser fields, while they remain unchanged when these quantities change according to the scaling law. These results verify the scaling law.

This paper is arranged as follows: the numerical method is given in Section 2. The effects of binding energy, wavelength, laser intensity, and the combined effect of the three quantities on photoelectron energy spectra are presented in Section 3, with some discussion on the spectra. Section 4 ends with the conclusion.

2. Numerical method

The TDSE method has been extensively used in dealing with the interaction process of atoms and molecules with intense laser fields. Many authors have used this method to explain experimental observations and to disclose various physical processes of light-matter interaction.[18] One advantage is that it can mimic detailed conditions which are hard to treat analytically, such as the Coulomb effect neglected in the strong field approximation (SFA).[19] Thus, it was also used to examine the validity of the analytical conclusions. In our simulation, with the single active electron approximation, the three-dimensional TDSE for an atom interacting with a linearly polarized laser field is given by (in atomic units)

$$\mathrm{i}\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t)=(-\frac{1}{2}\boldsymbol{\nabla}^2+V(\boldsymbol{r})-\mathrm{i}\boldsymbol{\nabla}\cdot\boldsymbol{A}(t))\Psi(\boldsymbol{r},t), \quad (1)$$

where $\boldsymbol{A}(t)$ is the vector potential of the laser field, $V(\boldsymbol{r})$ is the Coulomb potential, and the velocity gauge is used. The wave function is expanded in spherical harmonics and on the radial-position angular-moment grid

$$\Psi(\boldsymbol{r},t)=\sum_{l=0}^{l_{\max}}\frac{1}{r}R_l(r)Y(\Omega), \quad (2)$$

where $\boldsymbol{r}$ is the position vector of the electron and $r\equiv|\boldsymbol{r}|$, $R_l(r)$ is the radial wave function, and Ω is the solid angle of $\boldsymbol{r}$. The magnetic index m is suppressed since the linearly polarized laser pulse is used. The detailed numerical algorithm and propagation scheme are presented in Ref. [20]. The Coulomb potential takes the form

$$V(\boldsymbol{r})=-\frac{1}{r}(Z+a\exp(-br)), \quad (3)$$

where Z is the nuclear charge number. By adjusting parameters a and b, we obtain the ground energy of various target atoms. For example, $a=0$ $(Z=1)$ corresponds to the ground state of hydrogen atoms, while $a=17.0$ and $b=19.83$ build a model atom with binding energy $E_\mathrm{b}=20.4$ eV. The radial grid includes 8000 points with grid spacing $\Delta r=0.1$ a.u. and 30 angular momenta are involved. In order to avoid the influence of the pulse shape, a ten-cycle trapezoidal pulse with a half-cycle in the rising edge and the falling edge is employed.

The code begins from the ground state of target atoms obtained by the widely-used imaginary time propagation and thereafter propagates with the laser pulse being switched on. When the laser pulse is switched off, we obtain the final state of the interacting system $\Psi(t_\mathrm{f})$. The energy-resolved photoelectron spectrum that we mainly focus on is achieved by[21]

$$P_\gamma(\mathscr{E})=\langle\Psi(t_\mathrm{f})|W_\gamma^2(\mathscr{E})|\Psi(t_\mathrm{f})\rangle, \quad (4)$$

with

$$W_\gamma(\mathscr{E})=\frac{\gamma^{2^n}}{(H_0-\mathscr{E})^{2^n}+\gamma^{2^n}}, \quad (5)$$

where H_0 is the non-field Hamiltonian, γ is the half width of the energy window, and n is the order of the window operator and is set to be 3 in our calculations. The width of the energy window is set to be 0.01 a.u.

3. Results and discussion

The scaling law states that the photoelectron energy spectrum for an atom with binding energy KE_b, shined by a laser beam of frequency $K\omega$ and intensity K^3I has the same shape as that for an atom with binding energy E_b, shined by a laser beam of frequency ω and intensity I, but the former is K times the latter in the photoelectron yield.[14] We also say, under a scaling transformation which maps (E_b,ω,I) to $(KE_\mathrm{b},K\omega,K^3I)$, the photoelectron energy spectra in a logarithmic scale are invariant but subjected to a constant magnitude difference $\log K$.

Photoionization of atoms depends on many factors, such as the binding energy of target atoms, the intensity and the frequency of driving laser fields. The scaling relationship between the laser frequency and the atomic binding energy is trivial, while the cubic relationship pertinent to the laser intensity is the key of the scaling law and is highly nontrivial. In order to verify the scaling law, we first show the variation of the photoelectron energy spectra when only one of these physical quantities changes, to figure out what trend it will be, then

change simultaneously all the related quantities to show the variation of photoelectron energy spectra.

Firstly, we studies the photoelectron energy spectra when only one quantity changed. Some results are depicted in Fig. 1. Figure 1(a) shows the photoelectron energy spectra of the hydrogen atom and a model atom with $E_b = 20.4$ eV irradiated by laser pulse of wavelength 800 nm and intensity 2×10^{14} W/cm^2. Both the energy spectra exhibit the plateau structure following a falloff in the low-energy part and followed by a sharp cutoff in the high-energy part. The photoelectron yield of the hydrogen atom is generally higher than that of the model atom by more than two orders of magnitude. Because the ponderomotive energy U_p is constant, the cutoff energy is the same. Figure 1(b) shows two calculated photoelectron spectra of the hydrogen atom irradiated by a laser field with constant intensity but different wavelengths. The pronounced difference between them is the length of the plateau. The photoelectron energy spectrum from a 900-nm laser has a much wider plateau than that from a 700-nm laser. This is caused by the ponderomotive energy that is quadratically dependent on the wavelength, therefore the photoelectrons gain more quiver energy in the longer wavelength laser field. Figure 1(c) depicts two spectra of the hydrogen atom by different laser intensities for the same wavelength, from which we see the laser intensity affect the photoelectron yield and the plateau significantly. For an intensity of 1.0×10^{14} W/cm^2, the photoelectron energy spectrum exhibits a wider plateau up to more than 100 eV and the overall ionization yield is notably higher than the other one. This indicates that the laser intensity plays a dominant role in producing high-energy photoelectrons.

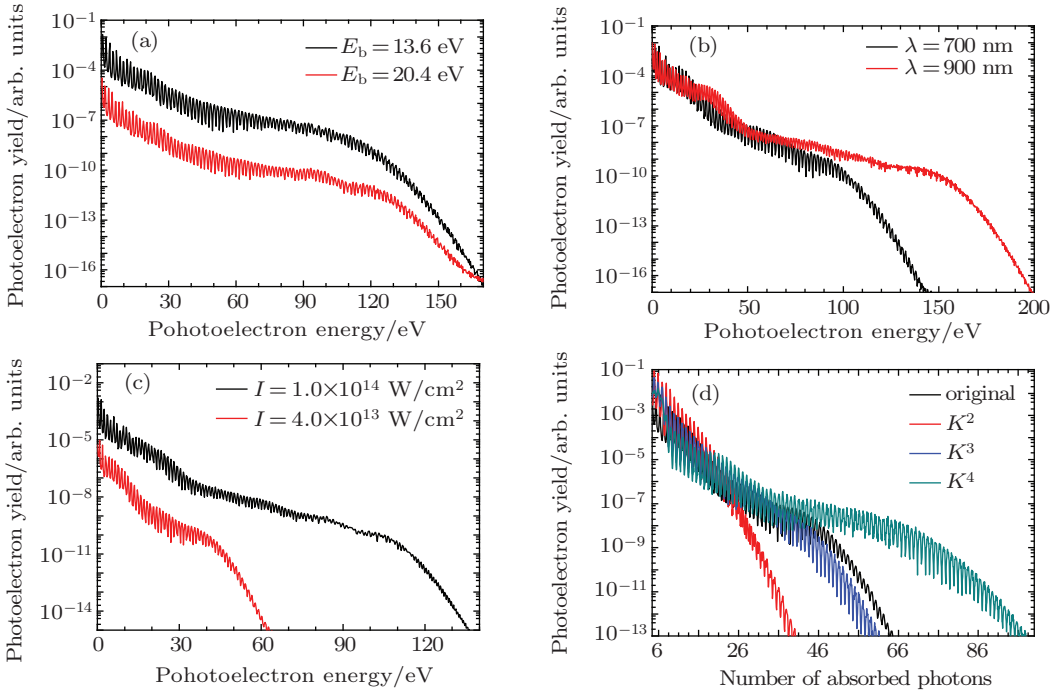


Fig. 1. (color online) Photoelectron energy spectra calculated for different atoms irradiated by different laser fields: (a) for hydrogen ($E_b = 13.6$ eV) and the model atoms ($E_b = 20.4$ eV) in a laser pulse of wavelength 800 nm and intensity 2.0×10^{14} W/cm^2; (b) for hydrogen atoms in laser pulse of intensity 2.0×10^{14} W/cm^2, but for wavelength 700 nm and 900 nm, respectively; (c) for hydrogen atoms in laser pulses of wavelength 1064 nm, but for laser intensity 1.0×10^{14} W/cm^2 and 4.0×10^{13} W/cm^2, respectively; (d) for hydrogen atoms in different laser fields: the original one is for a laser field with $\lambda_0 = 800$ nm, $I_0 = 1.0 \times 10^{14}$ W/cm^2; while others are for the wavelength λ_0/K and laser intensities $K^2 I_0$, $K^3 I_0$, and $K^4 I_0$, respectively, and $K = 2$.

Secondly, we show the photoelectron spectra with one quantity unchanged. Figure 1(d) depicts the spectra of a hydrogen atom irradiated by laser fields of different intensities and different wavelengths. For convenience of comparison, the horizontal axis employs the absorbed photon number and the spectrum marked by the black line shifts left by 4.5 such that the ATI peaks are in the same order. We see the shapes of the spectra are quite different from each other, even for the original spectra and for the one with intensity $K^3 I_0$. These significant discrepancies, especially in the cutoff region, reflect substantially that they are different ionization processes. We also simulate the other two cases, i.e., keeping wavelength or intensity unchanged and simultaneously altering the other two parameters. However, significant discrepancies are also found. Thus, we conclude that the photoelectron spectra cannot be the same when only two quantities change.

From the above discussions, we clearly see that the binding potential E_b, the wavelength λ, and intensity I of the laser field affect the photoelectron energy spectra in different ways. Increasing both I and λ prolongs the plateau of the photoelec-

tron energy spectra, while increasing I and decreasing E_b enhances the height of the spectra. Therefore, one may wonder whether the photoelectron energy spectra can be kept invariant if increasing I and E_b but decreasing λ in some special way. The answer lies in the scaling law.

The scaling law states that for atoms with different binding energies, for example if the binding energy enlarges K times, in order to keep the photoelectron energy spectra unchanged, the frequency of the driving laser field should be enlarged by K times and the laser intensity should be enlarged K^3 times. The reason for this is to keep the ponderomotive parameter $u_p \equiv U_p/\hbar\omega \propto I/\omega^3$ unchanged when the laser frequency changes. In order to check this scaling relationship, we do the following: first we choose the photoelectron energy spectrum of a hydrogen atom ($E_b = 13.6$ eV) irradiated by a laser pulse of wavelength 800 nm and intensity $I = 10^{14}$ W/cm^2 as the reference; then we calculate the photoelectron energy spectra of a model atom with binding energy KE_b irradiated by laser field of wavelength λ/K and intensity KI, K^2I, K^3I, and K^4I, respectively; finally we compare the calculated spectra for different K. One comparison with $K = 1.5$ is shown in Fig. 2. For convenience of comparison, the horizontal axis represents the number of absorbed photons, and the spectra for K and K^2 (K^4) are shifted down (up) by one order of magnitude, respectively. From this figure we see the photoelectron energy spectrum for K^3 agrees well with the original one, while others show more or less differences from the original one. Thus the scaling law of photoelectron energy spectra is verified by an independent method that is completely different from the original analysis. This indicates that the ponderomotive parameter is a vital parameter in the interaction of atoms with intense laser fields.

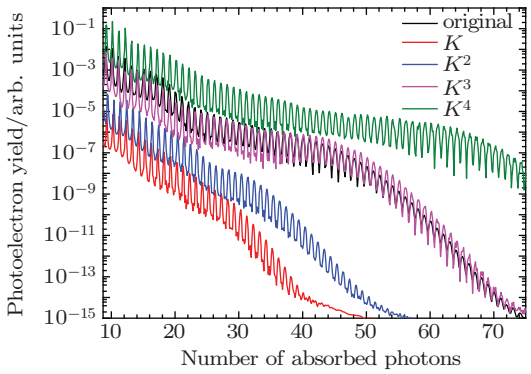


Fig. 2. (color online) Photoelectron energy spectrum denoted by the black line is for the hydrogen atom irradiated by a laser pulse of wavelength $\lambda_0 = 800$ nm and intensity $I_0 = 10^{14}$ W/cm^2. Other spectra are for the model atom ($E_b = 20.4$ eV) irradiated by laser pulses of wavelength $\lambda = 533.3$ nm and different laser intensities: 1.5 (K), 2.25 (K^2), 3.38 (K^3), 5.06 (K^4) $\times 10^{14}$ W/cm^2, respectively.

Detailed comparisons between the photoelectron energy spectrum for K^3 and the original one show that the yield of low-energy photoelectrons from the hydrogen atom is lower than that from the model atom, while for high-energy photoelectrons, the difference becomes the opposite case. This discrepancy becomes more distinctive for a larger K. According to our analytical results which are based on the SFA, the ionization rates of each photoelectron peak spectra are enlarged by K times under the scaling transformation. This feature agrees well with the TDSE results for high-energy photoelectrons, but not for low-energy photoelectrons. What causes the discrepancy?

The discrepancy may come from two sources, one is the initial wave function which is chosen as the hydrogen-like 1s states in the analytical studies, another is the attraction of parent core to the photoelectrons which is neglected in the analytical studies. The initial wave function determines the initial distribution of bound electrons and may affect the ionization rates when it projects on the final electronic states. The influence of the Coulomb attraction on low energy photoelectrons is strong but becomes weak on high-energy photoelectrons,[22] which may decrease the ionization yield of low-energy photoelectrons.

In order to seek for the origin of the discrepancy, we do the following: We change Z into $\sqrt{K}$ and set $a = 0$ in Eq. (3). In such a manner, the initial wave function is obtained as the hydrogen-like 1s state. We then calculate the spectra according to the scaling law for several K. Results are shown in Fig. 3, from which we see the overall shapes of the spectra agree perfectly well with each other, although numerical data disclosed that the yields of lower-energy peaks are not exactly enhanced by K times. This difference is caused by the attraction of binding potential to the photoelectrons which is neglected in the SFA.[22]

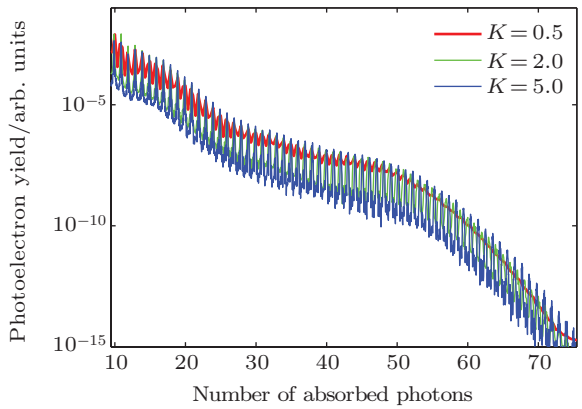


Fig. 3. (color online) Photoelectron spectra calculated according to the scaling law for three values of K. The initial wave functions are set as that of the hydrogen-like 1s state by changing Z as $\sqrt{K}$ times. The parameters of the benchmark spectrum (not shown) are chosen as: laser wavelength 800 nm and laser intensity 10^{14} W/cm^2, and for the hydrogen atoms.

Our calculations also show that the yield of lower-energy photoelectrons is greatly affected by the initial wave functions,

while it is not for higher-energy photoelectrons. This implies that the rescattered photoelectrons are less affected by the initial state of the bound electrons and are greatly dominated by the parent core during rescattering. In fact, the rescattered photoelectrons were regarded as free electrons and were used to detect the structure of the parent cores.[8–10,23]

4. Conclusions

By means of the numerical solution of TDSE, we calculated the photoelectron energy spectra of different atoms irradiated by various laser fields. We find that the photoelectron energy spectra related by the scaling law are the same, especially for high-energy photoelectrons, which verifies numerically that the scaling law that was concluded analytically. The verification of the scaling law by independent methods provides an incontestable support to the validity of the scaling law.

The scaling law has a wide usage in studies related with photoionization. The scaling law connects the photoelectron energy spectra, as well as the angular distributions, from atoms of different binding energies irradiated by laser fields of different frequencies and intensities, and thus provides a powerful and convenient tool to identify the equivalent physical process of atoms in various laser fields. The scaling law makes it easy for theoreticians to identify the equivalent physical process and provides an instruction for experimentalists to choose suitable and effective experimental conditions. The scaling law provides a reference in various usages of rescattered photoelectrons.

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