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Extracting the information of scattering potential using angular distributions of rescattered photoelectrons

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The rescattered photoelectrons are greatly affected by the binding potential of the parent core, while the directly emitted photoelectrons not. They are of comparable probability amplitudes at the onset of the plateau in the kinetic energy spectra of photoelectrons, which leads to the photoelectron angular distributions varying distinctively with the binding potential of the targets. We exhibit such variations and propose that the variations can be used to extract the potential information of the target core.

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High-order above-threshold ionization (ATI) is characterized by a broad plateau followed by a cutoff at about $10U_p$ in the photoelectron energy spectrum (PES) [1–3], where U_p is the ponderomotive energy. Generally, the generation of those high-energy photoelectrons is accounted by a so-called rescattering mechanism [4]: when irradiated by an intense laser field, the bound electrons of atoms or molecules are excited into continuum states. Intuitively, when the electric field of the incident laser reverses, some electrons in the continuum states may be pulled back to the vicinity of their parent cores. Then the attraction of their parent cores becomes the dominant factor that governs the subsequent motion of those driven-back electrons. Some of those electrons are rescattered then escape from the laser field. The photoelectrons arising from the rescattering process are of much higher kinetic energy, up to about $10U_p$, since they are further accelerated by the electric field. More importantly, the rescattered photoelectrons bring out the information about the potential of their parent core, thus provides a supplementary means to learn the core structure of the target atoms and molecules [5–7].

Many efforts have been contributed to that end. The ring structure in photoelectron angular distributions (PADs) of the ATI orders at the onset of the plateau was attributed to the rescattering effect [2, 8]. Milošević *et al.* showed the variation of the plateau with the screening parameter of the Yukawa potential and pointed out that the PES may be used to detect the binding potential of the target atoms [9]. Recently, Morishita *et al.* proposed that the momentum spectra of high-order ATI can be used to retrieve the core structure of the target atoms and molecules [10, 11].

In our recent analytical study based on the quantum scattering theory of ATI developed by Guo, Åberg and Creasmann [12], we reproduce the plateau structure of the PES and confirm that the high-order ATI is caused mainly by the rescattering effect of the parent core. We find that the ionization amplitude includes two parts: one is formed by the directly emitted photoelectrons in which the influence of the parent core is included only in the initial wave function, while the other is formed by the rescattered photoelectrons and depends explicitly on the binding potential of the parent core. The emission rate from the direct ionization decreases rapidly as the ATI order increases, while that from the rescattering process changes gently up to a sharp cutoff at about $10U_p$. At the onset of the plateau, the photoelectrons coming from two sources have comparable probability amplitudes, thus their interference effect is strong, consequently, any variation of the rescattered photoelectrons becomes evident. This finding discloses the possibility to extract the information about the potential of the core by the rescattered photoelectrons, especially by the photoelectrons at the onset of the plateau structure. Such a scheme has unique advantages which were not disclosed by other related studies.

In this paper, we demonstrate that the PES and the PADs at the onset of the plateau are very sensitive to the binding potential of the parent core, thus can be used to extract the information of scattering potential. The angular distributions of photoelectrons in the rest part of the spectrum do not meet that end, although their absolute values also depend on the binding potential of the parent core. In order to exhibit the variation of the PES and the PADs, we take two widely used model potentials as examples, i.e. the Yukawa potential and the Gaussian potential. We believe that the phenomena demonstrated here can be easily expanded into other model potentials, which provides an important reference in extracting the information of scattering potential by the rescattered photoelectrons.

In our analytical study, we use standard perturbation theory to derive an expression for the photoelectron ionization rate. Using the quantized-field Volkov states as the intermediate states [12], we ob-

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tain the differential ionization rate for a given ATI order as (the units $\hbar = c = 1$ are used)

$$\frac{dW}{d\Omega_{p_f}} = \frac{(2m_e^3\omega^5)^{1/2}}{(2\pi)^2}(q-e_b)^{1/2}|T_d+T_r|^2, \qquad (1)$$

where $d\Omega_{p_f} = \sin\theta d\theta d\phi$ is the solid angle in the momentum space, in which θ is the scattering angle and ϕ is the azimuth angle; m_e is the rest mass of the electron and q is the number of photons absorbed during the overall ionization process and denotes the ATI order. The kinetic energy of photoelectrons satisfies

$$E_k \equiv \frac{\mathbf{P}_f^2}{2m_e} = q\omega - e_b\omega, \qquad (2)$$

where $\mathbf{P}_f$ is the final momentum of photoelectrons and $e_b\omega$ is the binding energy of the target atom. The first transition matrix element in Eq. (1) is for the directly emitted photoelectrons [12]

$$T_d = (u_p - j_i)\mathcal{X}_{-j_i}(\zeta_f,\eta)^*\mathcal{X}_{-j_f}(\zeta_f,\eta)\Phi_i(|\mathbf{P}_f - q\mathbf{k}|), \qquad (3)$$

in which $u_p = U_p/\omega$ is the ponderomotive parameter, j_i and j_f are the numbers of absorbed photons in the excitation and the exit processes, respectively. The quantity $\Phi_i(|\mathbf{P}|)$ is the Fourier transform of the wave function of the initial bound electron, which depends on the binding potential of the target core. The second transition matrix element in Eq. (1) can be described by

$$\begin{aligned} T_r \propto -i\pi \sum_{\mathcal{E}_{\mathbf{P},n}=\mathcal{E}_f}\ \sum_{\mathcal{E}_{\mathbf{P}',n'}=\mathcal{E}_{\mathbf{P},n}} \langle \phi_f, n_f | \Psi_{\mathbf{P},n}\rangle \qquad (4) \\ \times \langle \Psi_{\mathbf{P},n} | U | \Psi_{\mathbf{P}',n'}\rangle \langle \Psi_{\mathbf{P}',n'} | V | \Phi_i, n_i\rangle , \end{aligned}$$

where V is the interaction operator between the electron and the laser field, U denotes the attraction of the ionic core to the electron; The quantity $\mathcal{E}_{\mathbf{P},n}$ is the eigen energy of the quantized-field Volkov state $|\Psi_{\mathbf{P},n}\rangle$, in which $\mathbf{P}$ is the momentum of the electron and n is the number of background photons [12]. The summations are performed over all the Volkov states with the same eigen energy. The first factor of Eq. (4), from the right, describes the excitation of the initially bound electron to a Volkov state under the action of the laser field, and the third factor describes the exit process of the electron from the Volkov state to the final plane wave state, while the second factor describes the transition from a Volkov state to another on-energy-shell Volkov state under the attraction of the ionic core. Thus T_r term describes the rescattering amplitude of on-energy-shell transitions. It is worked out to be

$$\begin{aligned} T_r = \frac{im_e}{4\pi^{3/2}} \sum_{j_i} \mathcal{X}_{-j_f}(\zeta_f,\eta)(u_p - j_i)|\mathbf{P}|\Phi_i(|\mathbf{P}|) \qquad (5) \\ \times \int d\Omega_{\mathbf{P}} X_{q-j_i+j_f}(\zeta-\zeta_f)\mathcal{X}_{-j_i}(\zeta,\eta)^* U(\mathbf{P}_f - \mathbf{P} - q\mathbf{k}) \end{aligned}$$

where $|\mathbf{P}| = (2m_e\omega)^{1/2}(j_i - u_p - e_b)^{1/2}$, and $U(\mathbf{P})$ is the Fourier transform of the binding potential. In our calculations, we set u_p equal to j_f [12]. The (generalized) phased Bessel functions are defined as [13]

$$\begin{aligned} X_n(z) &\equiv J_n(|z|)e^{in\arg(z)}, \qquad (6) \\ \mathcal{X}_j(z,z') &\equiv \sum_{m=-\infty}^{\infty} X_{j-2m}(z)X_m(z'), \end{aligned}$$

where z and z' are complex variables and the arguments in Eqs. (3) and (5) are given by

$$\zeta_f = \zeta_0\mathbf{P}_f\cdot\boldsymbol{\epsilon}, \quad \zeta = \zeta_0\mathbf{P}\cdot\boldsymbol{\epsilon}, \;\; \eta = u_p\boldsymbol{\epsilon}\cdot\boldsymbol{\epsilon}/2, \qquad (7)$$

where $\zeta_0 = 2\sqrt{u_p/(m_e\omega)}$ and $\boldsymbol{\epsilon}$ is the polarization vector of the laser beam.

From the transition matrix elements, we see for the directly emitted photoelectrons, the effect of binding potential only exists in the initial wave function. Although in the ionization process the parent core may affect the photoelectrons more or less, generally, the effect is weak compared with that of the intense laser field. This is the physical origin of the widely used strong field approximation. While, for the rescattered photoelectrons, besides the initial wave function, the convolution of the binding potential $U(\mathbf{P}_f - \mathbf{P} - q\mathbf{k})$ also appears explicitly in the transition matrix. This implies that the effect of the binding potential is accumulated during the rescattering process. This effect becomes more important when the photoelectrons move in the vicinity of the parent core. As a result, the subsequent motion of the rescattered photoelectrons is implanted the information about the potential of the target atoms. Thus, using the rescattered photoelectrons to acquire the core information attracted much attentions by the end of last century. Several observables, such as the PES and the momentum distributions, were used to extract the structure information of the targets [10, 14]. Our study shows that the angular distributions of the photoelectrons at the onset of the plateau in PES provide a convenient tool to that purpose. The advantage of using the PADs lies in the fact that the shape of PAD indicates the relative variation of the ionization rate and that the PADs can be easily and exactly detected in experiments. The reason to use the PADs at the onset of the plateau is as follows: For low-energy photoelectrons, generally with kinetic energy less than $2U_p$, they are mainly directly emitted thus take less information of the parent core. In the onset region of the plateau, generally with kinetic energy about $2U_p$, both the directly emitted and the rescattered photoelectrons are of comparable probability amplitudes thus the interference becomes evident. Since the directly emitted photoelectrons are affected less by the core, any trivial difference in the rescattering amplitudes will greatly change the PADs, thus the PADs become very sensitive to the binding potential of the parent core. For photoelectrons with energy far larger than $2U_p$, however, the PADs become less dependent on the binding potential, since the photoelectrons come mainly from the rescattering process and the binding potential just provides a common factor related to the emission rate.

In analytical calculations, the model potentials are commonly used to mimic the real potential which is determined by the inner electron distribution and can not be described by the Coulomb potential simply [9]. By adjusting the parameters of the model potentials, the real potential is described more accurately. In the following, employing the Yukawa potential and the Gaussian potential, we calculate the energy spectra and angular distributions of photoelectrons to show their variation with the parameters of the model potentials. The Yukawa potential can be expressed as [15]

$$U_Y(\mathbf{r}) = -\frac{Ze^2}{4\pi r}\exp(-\lambda r), \tag{8}$$

where Z denotes the number of charge in the ionic core, λ is the screening parameter, which can be changed to suit different ionic binding potentials. Once $r \geq 1/\lambda$, the potential goes rapidly to zero; when $\lambda \to 0$, the Yukawa potential becomes the Coulomb potential, thus it is also called the screened Coulomb potential. Its Fourier transform is worked out to be

$$U_Y(\mathbf{P}) = -\frac{Ze^2}{|\mathbf{P}|^2+\lambda^2}. \tag{9}$$

The variation of this potential is performed by changing the value of λ. The Gaussian potential is given by [16]

$$U_G(r) = -U_0\exp(-r^2/r_0^2), \tag{10}$$

where the parameter U_0 mainly determines the height of the potential well and r_0 mainly determines the gradient of the potential well. The Fourier transform is worked out to be

$$U_G(\mathbf{P}) = -U_0 r_0^3\pi^{3/2}\exp(-|\mathbf{P}|^2 r_0^2/4). \tag{11}$$

The variation of this potential is performed by changing the value of r_0. In the following we will show the variation of PADs with those parameters. The wave function is chosen as that of the hydrogen-like 1s state. The driving laser field is linearly polarized and of wavelength 800 nm and intensity 1.5×10^{14} W/cm^2. In our calculations, we set the scattering angle $\theta = \pi/2$, and the PAD is obtained by varying the azimuth angle ϕ from 0 to 2π.

The calculated PES and PADs using the Yukawa potential for several values of the screening parameter are shown in Figs. 1 and 2, respectively. From Fig. 1 we see that each PES exhibits a plateau following the falloff at low-energy region and followed by a cutoff at about $10U_p$. As the screening parameter decreases, the height and the width of the plateau increase. Physically, a smaller screening parameter implies the attraction of the parent core to the photoelectrons decreasing slowly, i.e. the attraction of the parent core affects a relatively large range,

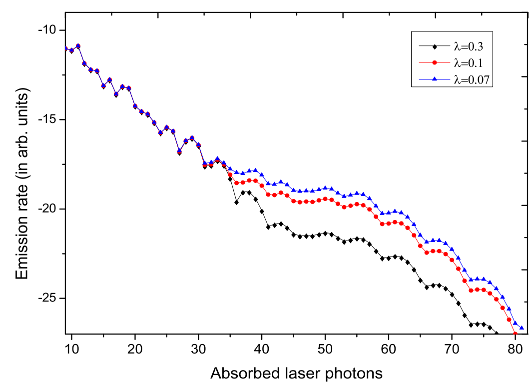

FIG. 1: (Color online) The calculated energy spectra for photoelectrons rescattered by the Yukawa potential with several screened parameters. We set Z =1.

thus more photoelectrons are rescattered. However, the cutoff of the plateau is independent of the screening parameter, since the maximal kinetic energy of photoelectrons is determined mainly by the laser field. Such variation in PES was also demonstrated by Milošević *et al.* using the generalized Keldysh-Faisal-Reiss theory [9].

Figure 2 depicts the variation of PADs with the screening parameter. The PADs in each row are of the same ATI order, but for different λ. We see that the PADs in the onset of the plateau change significantly with the screening parameter, while not for the photoelectrons in the falloff region of PES and those in the rest part of the plateau. The PADs shown in the top row are for the 28th ATI order which is formed mainly by directly emitted photoelectrons. We see that the PADs are of the same shape, and the difference is a common factor which depends on the emission rate. The PADs shown in the bottom row are for the 45th ATI order, which is formed mainly by the rescattered photoelectrons. The PADs are of the same shape and change less with the screening parameter, too. Other PADs are for the photoelectrons in the onset of the plateau, and their shapes vary with the screening parameter distinctively for the same ATI order. Milošević *et al.* also studied the angular distributions of rescattered photoelectrons but in the cutoff region, and they ascribed the rings of PADs to the cutoff of the plateau [9].

The variation of PADs with the binding potential of the parent core is not only limited to the Yukawa model potential and does not hold only for hydrogen-like atoms. It is a general feature resulted from the physical origin of the rescattering process. In order to show its generality, we take another widely used model potential, the Gaussian potential, to show the dependence. In Figs. 3 and 4 we depict the calculated PES and the PADs using the Gaussian potential for several values of r_0. As the parameter r_0 increases, the height and the width of the plateau increase. Since r_0 mainly determines the gradient of the potential well and a smaller parameter r_0 im-

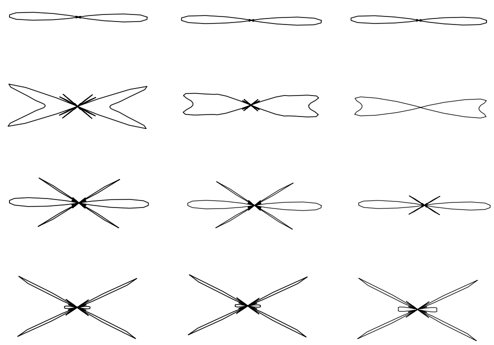

FIG. 2: Polar plots of the PADs calculated using the Yukawa potential. The PADs from the top to the bottom row are of the 28th, 35th, 42nd, and 45th ATI, respectively. The screening parameter in each column is set as 0.07 (left), 0.1 (middle) and 0.3 (right), respectively.

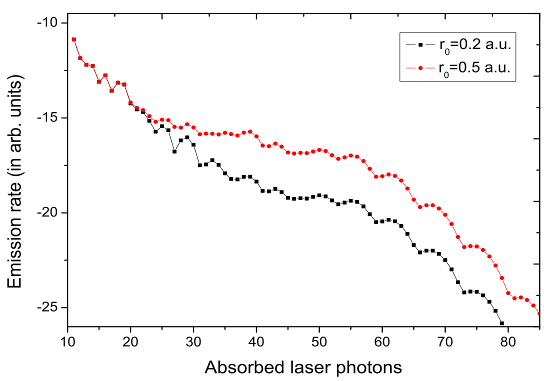

FIG. 3: (Color online) The calculated energy spectra of photoelectrons rescattered by the Gaussian potential with several r_0. We set $U_0 = 60$ eV.

plies a steeper potential well, a bigger r_0 means a larger range affected by the parent core and then more photoelectrons are rescattered. Consequently, the plateau becomes higher and wider, as shown in Fig. 3. Several PADs are depicted in Fig. 4. We see the PADs of the 15th and those of the 40th ATI orders are almost identical for different r_0, respectively, while the PADs in the onset of the plateau (e.g. the 30th) vary with r_0 significantly. The results for the Gaussian potential are qualitatively the same as those for the Yukawa potential.

How to extract the information of scattering potential for a given atom by the rescattered photoelectrons from the experimental data? In order to do this, one needs a reference that is obtained by theoretical calculations of the atoms with the same binding energy and the known wave function irradiated by the identical laser field. The differences between the experimental data and the model calculations originate from the different core structures. In performing the model calculations, one may use the

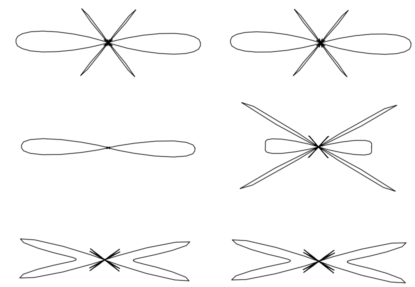

FIG. 4: Polar plots of the PADs calculated using the Gaussian potential. The PADs in the first, second and third rows are for the 15th, 30th and 40th ATI, respectively. The value of r_0 for the left and right columns is set as 0.2 and 0.5, respectively.

scaling law of rescattered photoelectrons [17, 18].

In summary, the photoelectrons of high-order ATI come from two sources, one is the directly emitted photoelectrons and the other is rescattered photoelectrons. The rescattered photoelectrons are greatly affected by the binding potential of the parent core, while the directly emitted photoelectrons not. They are of comparable probability amplitudes at the onset of the plateau in PES. This leads to the PADs at the onset of the plateau varying distinctively with the binding potential of the target atoms. In this paper, we exhibit the variations of the PADs with the binding potential and propose that such variations can be used to extract the information of scattering potential of the target core.

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