Space distribution of the rescattering electron wavepacket in the laser-atom interactions

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Abstract. We investigated the space distribution of the rescattering electron wavepacket created in the laser-atom interaction by a full quantum simulation and a semiclassical calculation. Both the quantum simulation and the semiclassical calculation showed that the rescattering electron beam current intensity can reach the order of 10⁹ A/cm², much intense than the conventional electron beam. Different from the convention electron beam, the rescattering electron beam is of a non-uniform distribution both in energy and space. The simulated information is important for analyzing the molecular structure in the rescattering imaging experiments.

The laser-material interaction is a hot research topics owing to the rapid advance of the laser technology. Most of the observed phenomena can be explained by the rescattering model proposed by Corkum [1]. The electron is firstly released by the laser through tunneling ionization when the laser field reaches its peak and the released electron is bounced back when the laser field changes the polarization direction. The collision of the bounced back electron with the parent core is similar to an electron beam incidents on the target. In principle, all the dynamics, which can be investigated by the conventional electron beam, can also be investigated with the rescattering electron beam. More attractively, the rescattering electron beam is a coherence beam and the beam intensity is much higher than the conventional one. Thus, the rescattering electron beam provides a potential way to image the molecular structure [2], like the conventional (e,2e) experiment [3]. For the conventional electron beam, the beam intensity, beam energy and so on can be controlled in the experiment. For the rescattering electron beam, the full information about the rescattering beam, namely, the energy distribution and the space distribution, is unknown. Without such knowledge, the beam quality cannot be controlled experimentally. Since the rescattering is an intermediate process, the information cannot be obtained directly from the experimental measurement. It has to rely on the numerical simulation.

In principle, all the dynamic information can be obtained by solving the time-dependent Schrödinger equation. In practice, directly getting the rescattering information is not easy because (1) the wavefunction corresponds to the tunneling ionized electron is just a small factional part of the total wavefunction; (2) the rescattering electron wavepackets created at different laser cycles mix up and so it is difficult to decompose the n-th returns clearly. Of course,
the rescattering information can be obtained by a semiclassical simulation [3] but the reliability of the classical results is not clear. In our previous work [3], we proposed a numerical procedure to obtain all the rescattering information directly by solving the time-integral equation instead of the differential Schrödinger equation and we extracted all the rescattering information. So far most of the works focused on the returning time and energy distribution, there is no report on the space distribution of the scattering electron, which is another crucial information for the molecular structure imaging study using rescattering electron beam. In this paper, we study the space distribution of the rescattering electron beam in a full quantum, nonperturbative method.

Similar to our previous work [3], we rewrote the time-dependent Schrödinger equation into an integral equation and factored out the non-active part which corresponds to the initial state without interacting with the laser field. The time-dependent wavefunction is formally written as (atomic units $\hbar = m = e = 1$ are used)

$$\Psi(t) = -i \int_{t_0}^{t_1} e^{-i \int_0^t [H_0 + V(t')] dt'} V(\tau) e^{-i H_0 \tau} \Phi_0 d\tau. \quad (1)$$

Here $\Phi_0$ is the initial state, $H_0$ is the laser-field free Hamiltonian (we took the hydrogen atom as an example) and $V(t) = -z E_0 \cos \omega t$ is the laser-electron interaction. $\Psi(t)$ is interpreted as the time dependent wavefunction due to the interaction of the atom with laser field during the time interval from $t_0$ to $t_1$, with $E_0$ the laser field peak strength and $\omega$ the laser frequency. Note that the exponential operator is a time-ordered operator. The time-propagation is performed by the split-operator method with a generalized pseudospectral grid in the energy representation [7, 8]. The laser-atom interaction $V$ appears twice in the above equation. The intuitive physical picture is that the atom is ionized due to the laser-atom interaction $V(\tau)$ and the ejected electron is propagated in the atomic field combined with the laser-atom interaction $V(t')$. At time $t$, we calculated the component of a given energy $E$ and partial wave $l$ of the laser-field free wavefunction in the inner region (collision region) as $C_l(E,t)$. With the coefficients $\{ C_l(E,t) \}$, we obtained the energy distribution of the rescattering electron wavepacket as

$$\frac{dP(E,t)}{dE} = \sum_l |C_l(E,t)|^2. \quad (2)$$

Because in the quantum mechanics, the impact parameter $b$ is not well defined, we approximate it as $b^2 = l(l+1)/(2E)$ and define the rescattering beam intensity as

$$I(b,t) = \frac{dP(b,t)}{2\pi b db} = \int \sum \frac{\sqrt{2E}}{\pi} |C_l(E,t)|^2 \delta \left( b^2 - \frac{l(l+1)}{2E} \right) dE. \quad (3)$$

In the present simulation, we chose the laser peak intensity $10^{14}$ W/cm$^2$ and wavelength 800 nm (the parameters most commonly used in the experiments). The tunneling ionization happens within half cycle from $\omega t_0 = -\pi/2$ to $\omega t_1 = \pi/2$. We traced the electron wavepacket when the ionization process is over. The upper panel in Fig. 1 shows the rescattering electron beam intensity $I(b,t)$. To compare with the conventional electron beam intensity, we converted the rescattering electron beam intensity from atomic unit to A/cm$^2$. The rescattering electron revisits the parent core at the returning times well predicted by the simple classical model [1] and the electron beam intensity reaches as high as $10^9$ A/cm$^2$, which is several orders intense than the electron beam intensity in the electron beam ion trap [9], which is of the order of $10^3$ A/cm$^2$. Note that the beam intensity obtained in the present work is about two orders smaller than the one predicted from the simple model [10]. The space distribution is not smooth but contains several strips within a given return time. These strips come from the discretized angular momenta. The most left one on the upper panel in Fig. 1 corresponds to the first
Figure 1. The rescattering electron beam intensity as a function of the rescattering time and the impact parameter $b$ from the quantum calculation (upper panel) and the rescattering energy and time distributions. The color coding represents the relative value of $\frac{dP(E,t)}{dE}$ (lower panel).

return, then the second one, the third one and so on. The space distribution is rather smooth, or uniformly distributed for the first return. At the third return, the electron is concentrated to the inner region, which corresponds to the close collision with the parent core. We attributed this to the Coulomb focusing effect. To explain the Coulomb focusing effect, we showed the time-dependent energy distribution of the rescattering electron on the lower panel in Fig 1. The rescattering energy reaches highest for the first return. The Coulomb focusing effect is less important for the high energy electron since it spends a less time in the inner region. When the electron returns to parent core again (the second return), the electron energy is much lower than the first return energy and the returning electron beam is focused due to the electron parent core Coulomb interaction. The focused electron moves along the laser polarization direction in a narrow region on the perpendicular plane to the polarization direction. When the focused electron beam is bounced back by the laser field with a relatively high energy in the third return, the Coulomb force does not affect the motion of the returning electron significantly. But the electron has already been focused in the small region on the plane perpendicular to the polarization direction during the second return. Thus the Coulomb focusing effect in the second return results in a high intensity electron beam at the third return.

With the understanding of the detail of the Coulomb focusing, let us revisit the rescattering induced double ionization experiments [10, 11, 12] of H$_2$ molecules. The strong third return peak was explained due to (a) the vibration wavepacket moves to the large $R$, the nuclei separation, results in a small ionization potential; (b) the third return energy is lower than the first return energy and closer to the ionization threshold or the peak position of the electron impact ionization cross section [13, 14]. From the present study, we know the Coulomb focusing
Figure 2. The rescattering electron intensity as a function of the rescattering time and the impact parameter \(b\) from the semi-classical simulation.

at the second return also contribute to the enhancement of the kinetic energy release at the third return. In the previous semi-classical simulations \([13, 14]\), such an effect was taken into account in the simulation without analysis in detail.

To cross check the reliability of the quantum calculation, we also performed a semi-classical simulation \([5]\). In the simulation we monitored the impact parameter \(b\)-dependent rescattering electron beam intensity as shown in Fig. 2. The electron beam intensity distribution is rather smooth because of the nature of the classical behavior. The obtained results are consistent with the quantum simulated ones both in the returning times and the beam intensity. The Coulomb focusing effect on the third return is also clearly seen. The major physical conclusions, like the smooth space distribution for the first return, are consistent in both calculations.

To summarize, we studied the rescattering electron space distribution when it revisits the parent core. The rescattering electron beam intensity can reach as high as \(10^9 \text{A/cm}^2\), which is much higher than the convention electron beams. With the understanding of the rescattering electron beam, it may help us to analyze the molecular electronic structure, analog to the conventional \((e,2e)\) experiment.

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