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Interpretation of momentum distribution of recoil ions from laser-induced nonsequential double ionization by semiclassical rescattering model

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Using a semiclassical rescattering model, the momentum distribution of recoil ions from laser-induced nonsequential double ionization is obtained and the result is consistent with the experiment reported recently. We show that the characteristic double-hump structure of the recoil momentum distribution of the He^{2+} ion parallel to the polarization axis is just the consequence of the rescattering dynamic of nonsequential double ionization and the acceleration of the ions in the laser field.

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The study of the interaction of atoms with intense laser fields has led to a comprehensive understanding of the nonlinear physics in the underlying dynamics of ionized electrons [1]. This advance was driven by significant progress in both experimental and theoretical capabilities. The recognition of the rescattering process and its leading to phenomena [2–4] was one of the most important steps in a complete understanding of the atom in laser fields. In fact, this thinking merely comes from a simple quasiclassical notion: Once an electron in a strong field has undergone a transition into continuum from its initial bound state, its motion is dominated by its interaction with the laser field. In the case of a linearly polarized field, a majority of these electrons will be driven back into the vicinity of the ion core and undergo elastic or inelastic scattering, or be recaptured into the ground state by emitting a high-energy photon. This process is the so-called rescattering process. Now, it is commonly believed that rescattering is responsible for many unusual observations, such as the cutoff law in high-order harmonic generation, a plateau formed by high-order ATI peaks, and the singular angular distributions of the photoelectrons in the plateau regime [2–10].

In recent years, double ionization of He or Ne in intense laser fields has gained more and more attention. It is well known that double ionization can occur either by a stepwise process or by a so-called nonsequential (NS) process. It is commonly accepted that in the stepwise process that occurs mainly above the saturation intensity for the single ionization (the intensity at which the neutral target atoms are fully depleted in the interaction volume), the electrons are ionized sequentially; i.e., its probability is characterized by the independent product of the probability of single ionization of the neutral atoms and that of the singly charged ions. In contrast, the mechanism of NS double ionization that occurs primarily in the intensity domain near and below the saturation intensity is still in debate [3,11–21].

Among the mechanisms that have been developed, three of them are rather important. Fittinghoff *et al*. suggested that the second electron could be shaken off by a nonadiabatic change of the potential caused by the emission of the first electron [11]. This mechanism is known to dominate double ionization of helium after absorption of single photons with energies beyond 1 keV [22]. The rescattering process has also been proposed to explain NS double ionization, first by Corkum [3]. In this model, the second electron is ionized in a collision with the first electron hitting its parent ion after free propagation during about half an optical cycle in the external laser field. Becker and Faisal proposed a ''correlated energy sharing'' model based on a so-called intense-field many-body *S*-matrix theory derived by a rearrangement of the usual *S*-matrix series [15,23]. This model includes short-time electron correlation (TS1) and the rescattering mechanism.

Recently, the measurements of the distributions of the recoil momentum of double charged He [24] and Ne [25] ions in the NS regime have been reported by two groups. There are several prominent features observed in both the experiments. First, a remarkable broad double-hump distribution at intensities near the saturation intensity for the recoil momentum parallel to the polarization direction, and a narrow single-hump distribution in the perpendicular direction; and second, there appears a cutoff recoil momentum in the parallel case, which is about $2\sqrt{4U_p}$ in the case of He [24], where U_p is the ''ponderomotive energy,'' i.e., the mean oscillation energy of a free electron in the laser field. It is believed that these characteristic features of the measured recoil momentum of the doubly charged ions can provide a test of the various models of NS double ionization. It has been pointed out in [24] that the measured He^{2+} momentum distributions are not consistent with that expected from the rescattering model. It is very interesting that, in contrast, the authors of [25] pointed out that, among the models, only the kinematics of the rescattering mechanism is in accordance with their experiment data.

In this paper, we calculate the recoil momentum of the doubly ionized ions of He by using a semiclassical rescattering model similar to that of Corkum [3]. The main purpose of this work is to see whether the rescattering model can give the distribution of the recoil momentum that is consistent with the experiment data.

First, we briefly present the semiclassical rescattering model adopted in our calculations. The ionization of the first electron from the bound state to the continuous state is treated by the tunneling ionization theory generalized by Delone and Krainov [26]. The subsequent evolution of the ionized electron and the bound electron in the combined Coulomb potential and the laser fields is described by a classical Newtonian equation. To emulate the evolution of the electron wave packet, a set of trajectories is launched with initial conditions taken from the wave function of the tunneling electron.

Evolution of the two-electron system after the tunnel ionization of the first electron is determined by the classical equations of motion (in atomic units)

$$\frac{d^2\mathbf{r}_i}{dt^2}=\mathbf{E}(t)-\boldsymbol{\nabla}(V_{ne}+V_{ee}). \tag{1}$$

Here $\mathbf{E}(t)=(0,0,F(t))$ is the electric field and $F(t)=F\cos(\omega t)$. The indices $i=1$ and 2 refer to the tunnel ionized and bound electron with ionization potentials I_{p1} and I_{p2}, respectively. The potentials are

$$V_{ne}=-\frac{2}{|\mathbf{r}_i|},\qquad V_{ee}=\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}. \tag{2}$$

The initial condition of the first, i.e., the tunneling electron is determined by a equation including the effective potential given in Ref. [27] and a generalized tunneling formula obtained by Delone and Krainov [26]. In parabolic coordinates, the Schrödinger equation for the first electron in a uniform field ϵ is written as

$$\frac{d^2\phi}{d\eta^2}+\left(\frac{I_{p1}}{2}+\frac{1}{2\eta}+\frac{1}{4\eta^2}+\frac{1}{4}\epsilon\eta\right)\phi=0. \tag{3}$$

The above equation has the form of a one-dimensional Schrödinger equation with the potential $U(\eta)=-1/4\eta-1/8\eta^2-\frac{1}{2}\epsilon\eta$ and the energy $K=I_{p1}/4$. The turning point, where the electron burns at time t_0, is determined by $U(\eta)=K$. In the quasistatic approximation, the above field parameter ϵ relates to the laser field amplitude $F(t)$ by $\epsilon=F(t_0)$.

The initial velocities are set to be $v_z=0,v_x=v_{per}\cos(\theta)$ and $v_y=v_{per}\sin(\theta)$. The weight of each trajectory is evaluated by [26]

$$\begin{aligned} w(t_0,v_{per})&=w(0)\overline{w}(1),\\ w(0)&=\frac{4(2I_{p1})^2}{\epsilon}\exp(-2(2|I_{p1}|)^{3/2}/3\epsilon),\\ \overline{w}(1)&=\frac{(2|I_{p1}|)^{1/2}}{\epsilon\pi}\exp(-v_{per}^2(2|I_{p1}|)^{1/2}/\epsilon),\end{aligned} \tag{4}$$

The initial condition of the second, i.e., the bound electron is determined by assuming that the electron is in the ground state of He^{1+} and its initial distribution is microcanonical distribution [28].

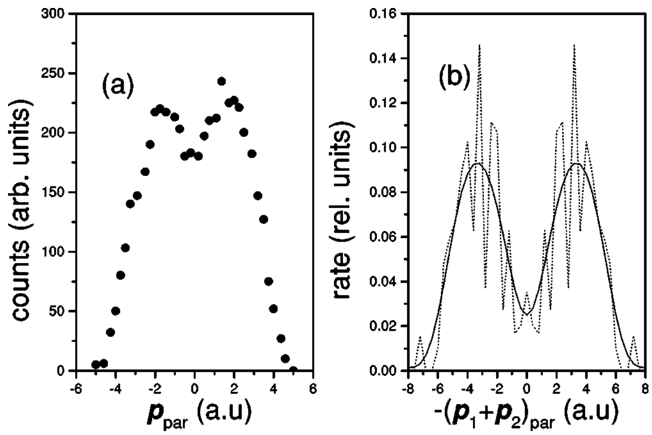

FIG. 1. Distribution of the recoil momentum of He^{2+} ions parallel to the polarization axis: (a) experiment; (b) dotted line, calculated result; solid line, after smoothing.

Compensated energy E_c advocated by Leopold and Percival [29] is introduced by

$$E_{ci}=\frac{m_e}{2}\left[\dot{\mathbf{r}}_i+\frac{e}{m_e}\int\mathbf{E}(t)dt\right]^2-2e^2/r_i. \tag{5}$$

When an electron is ionized completely, the Coulomb potential is weak enough and E_c tends to be a positive constant that is just the ATI energy in an ultrashort pulse laser.

Since the He^{2+} recoil momentum, $\mathbf{P}$, satisfies $\mathbf{P}\approx-(\mathbf{p}_1+\mathbf{p}_2)$ under the condition of the experiment [24], where $\mathbf{p}_1$ and $\mathbf{p}_2$ are momenta of the two ionized electrons, respectively, we need to calculate the distribution of the momentum of the two ionized electrons. The parameters in our calculation are chosen as $I_{p1}=0.9$ a.u. (24.12 eV), $I_{p2}=2$ a.u. (54.4 eV), $F=0.141$ a.u. ($I=6.6\times10^{14}$ W/cm^2) and $\omega=0.056\,42$ ($\lambda_1=800$ nm) corresponding to the experiment [24]. In the first step of our computation, 2×10^5 points are randomly distributed in the parameter volume $-\pi/2<\phi_0<\pi/2,v_{per}>0$ and $0<\theta<2\pi$ where $\phi_0=\omega t_0$. The trajectories are traced until at last one electron has moved to such a position that $r_i>200$. Finally, about 300 double-ionization cases are found in our calculation. Then these cases are traced until $t_f=13T$ to obtain the distribution of the momentum of the electrons. In the calculation, the field strength is a constant during $t_0<t<10T$ and is turned off in a cosine-squared shape during the last three periods.

Figure 1(a) shows the measured data for the recoil momentum of He^{2+} parallel to the polarization axis, obtained by Weber *et al*. [24]. Figure 1(b) shows the results of the present calculations. [Due to the symmetry of the field and the small value of the He^{2+}/He^{1+} rate, we choose $-\pi/2<\phi_0<\pi/2$ to search the double-ionization cases and calculate the distribution. The final distributions shown in Figs. 1(b) and 2(b) are obtained by reflecting the distribution relative to 0 and adding them together.] Comparison between these two figures shows that the essential features of the experimental distribution are reproduced qualitatively correctly by our semiclassical rescattering model. Both distributions show a characteristic double-hump structure with a

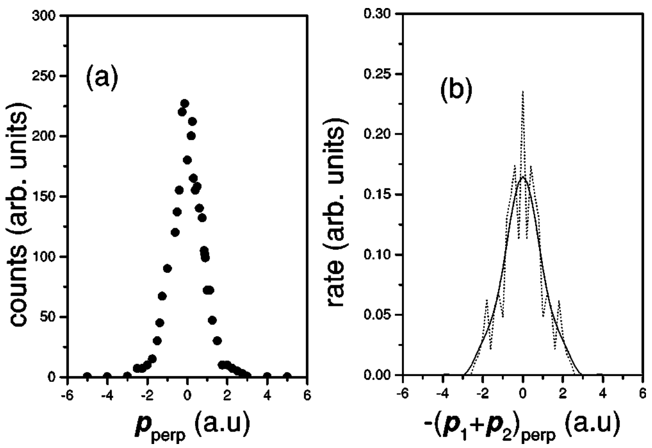

FIG. 2. Distribution of the recoil momentum of He^{2+} ions perpendicular to the polarization axis: (a) experiment; (b) dotted line, calculated result; solid line, after smoothing.

central minimum. The distributions of the perpendicular component of the recoil momentum are shown in Fig. 2. The essential features of the experimental distribution are again reproduced by the model. Both experiment and theory show a single-hump structure with qualitatively the same width. The calculated distribution of the parallel component [Fig. 1(b)] is found to be much broader than that of the perpendicular one [Fig. 2(b)]. This is also consistent with the experimental observation.

To study the origin of the two-hump structure of the distribution present in the parallel case, we show the trajectories of the tunneling electron in Fig. 3. Figure 3(a) shows a typical trajectory of the tunneling electron until the end of the pulse and Fig. 3(b) shows several trajectories of the electron that is still near the nucleus and interacts with the nucleus and the bound electron strongly. It should be pointed out that the sudden changes of the momenta in Fig. 3 indicate the collisions between the tunneling electron, the bound electron, and the nucleus. From Fig. 3, it can be concluded that the mechanism of the NS double ionization in the semiclassical rescattering model can be expressed as the following. First, the tunneling electron moves outward. When the direction of the field changes, the electron moves back to the ion and interacts with the nucleus and the bound electron. Second, if the kinetic energy of the tunneling electron is large enough when it comes back to the ion, the bound electron perhaps can be ionized and moves outward together with the tunneling electron. Thus, from the rescattering mechanism presented above, the origin of the characteristic two-hump structure of He^{2+} can be understood. For simplification, it can be assumed that only the electron that tunnels out at t_a has enough kinetic energy to ionize the bound electron when it moves back to the ion at time t_b (only consider $-T/4<t_a<T/4$ according to the symmetry of the laser field as stated above). It is also well known that the sum of the momentum of the two electrons after impact ionization is a single-hump distribution with central maximum without external field [30,31]. In the case with external field, the ionized electrons will be accelerated by the field. Then the maximum of the distribution of the sum of the momentum moves upward or downward (corresponding to $-T/4<t_a<T/4$ or $T/4<t_a<3T/4$) and finally forms a two-hump structure with central minimum.

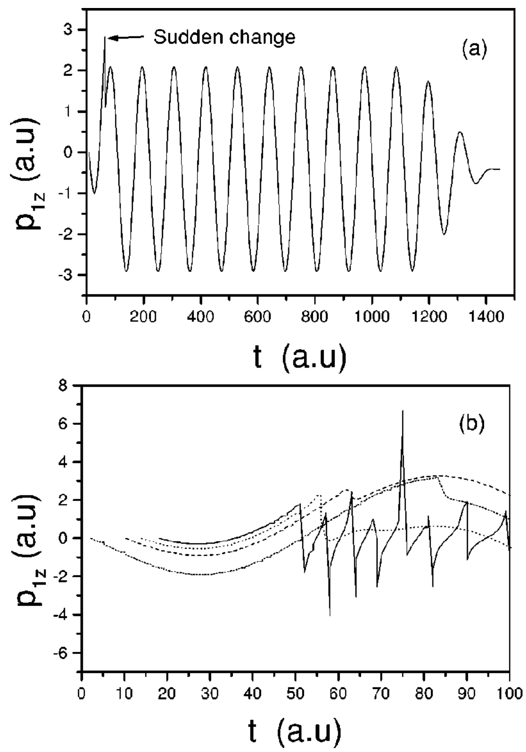

FIG. 3. Typical trajectories of the tunneling electron that lead to double ionization. (a) One whole typical trajectory; (b) trajectories near the ions.

During the work of this paper, we noted that Becker and Faisal gave an interpretation of the experimental data by using the ''correlated energy sharing'' model of the NS ionization [32]. A two-hump structure is also obtained by their quantum calculations and is qualitatively consistent with the experimental data. In our opinion, the consistency between the quantum theory and the semiclassical rescattering model is just because the ''rescattering'' process is also included in the ''correlated energy sharing'' model.

From Fig. 1, it is obvious that the distribution of the present calculation is somewhat broader than the experimental data, and the interval between the two maximums is also larger than that of the experimental data. These quantitative differences could be due to the uncertainty in the intensity measurements, the momentum resolution [24], and, maybe more important, that the semiclassical rescattering model is known to overestimate the rescattering effect since the rescattering process is treated classically without considering the quantum effects; e.g., the diffusion of the wave packet. Moreover, the simulation calculated here is different from the experiment in that only the tunneling electrons produced during the first period of the pulse are traced to obtain the distribution. This problem remains to be investigated in the future.

In conclusion, we have used the semiclassical rescattering model to calculate the momentum distribution of recoil ions from laser-induced nonsequential double ionization. The results obtained are consistent with the experimental data reported recently. It is shown that the characteristic double-hump structure of the recoil momentum distribution of the He^{2+} ion parallel to the polarization axis is just the consequence of the rescattering mechanism of NS double ionization and the acceleration of the ion in the laser field.

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