Double-plateau in the energy distribution of electrons scattered by ions-pairs in a strong laser field

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The energy distribution of electrons scattered from single ions and from pairs of ions in a strong laser field is studied in the framework of the one-dimensional time-dependent Schrödinger equation. For single ions, the properties of the scattering plateau are discussed as a function of the impact velocity. For pairs of ions, the existence of a double-plateau due to double-collisions is demonstrated and the dependence of its maximum energy on the ion distance is discussed. Potential applications to inverse bremsstrahlung absorption in plasmas and to ATI of diatomic molecules are indicated.

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I. INTRODUCTION

Rescattering in above threshold ionization (ATI) leads to the formation of a plateau in the energy distribution of the photo electrons. In the past, the structure of the ATI-plateau has been extensively studied in terms of classical, quasiclassical and quantum-mechanical treatments[1–7]. However, due to the specific conditions in the ionization problem, scattering has mostly been addressed in a limited range of impact velocities. In this work we consider scattering problems that extent the range of impact velocities leading to plateaus with considerably larger cut-off energies and to double-plateaus. The present calculations are based on numerical solutions of the one-dimensional (1d) time-dependent Schrödinger equation (TDSE) for wavepacket scattering from a softcore Coulomb potential in a laser field. For one ion, only one plateau can be observed, for two ions the existence of a second plateau due to double collisions can be demonstrated. The results can be explained in terms of the classical instantaneous collision model[8]. Potential applications to inverse bremsstrahlung (IB) absorption [9–17] and to ATI of diatomic molecules are discussed. A more detailed presentation of this work including an analytical solution of the energy distribution for instantaneous Coulomb collisions in three dimensions will be published elsewhere[18].

II. SCATTERING MODEL

As a model of electron-ion collisions, we consider scattering from a 1d-model potential. Similar 1d calculations have been performed in studies of electron capture[19, 20] and of scattering in the ATI regime[21]. Here we extent the range of impact velocities and calculate the energy distribution of the scattered electrons in both forward and backward direction. The polarization direction of the laser field is assumed parallel to the launch direction. Despite of the obvious simplifications in this model, the energy spectrum of backscattered electrons can be quite well understood in this framework and complete numerical solutions of the TDSE can be gained.

As a model potential, we choose a softcore Coulomb potential with charge state Z and cut-off distance ϵ,

$$V(x) = -\frac{Z}{\sqrt{x^2+\epsilon^2}}, \tag{1}$$

where all quantities are expressed in atomic units ($m = -e = \hbar = 1$, m: electronic mass, e: electronic charge, $\hbar$: Planck's constant). For scattering studies, a proper choice of the cut-off distance ϵ is crucial. For $\epsilon \gg 1$ the motion becomes quasiclassical and the reflectivity of the potential approaches zero. In the present numerical calculations we have therefore chosen the parameters $Z = 1$ and $\epsilon = 0.1$. It is noted that the present cut-off distance is much smaller than in previous work[19, 20] to account for collisions with impact parameters below one atomic unit (1 [a.u.]) in this model.

The laser field is described in the dipole approximation as a time-dependent electric field,

$$\mathcal{E}(t) = \mathcal{E}_0 \sin(\omega_0 t), \tag{2}$$

with amplitude $\mathcal{E}_0$ and frequency ω_0. Specifically, we set $\mathcal{E}_0 = 0.2$ and $\omega_0 = 0.2$. These parameters correspond to an intensity of $1.4 \cdot 10^{15}$ W/cm^2 and a wavelength of 0.23μm, respectively. The quiver velocity is $v_0 = \mathcal{E}_0/\omega_0 = 1.0$ and the ponderomotive potential

$U_p = v_0^2/4 = 0.25$. It is noted, that the typical energy of backscattered electrons, $(2v_0)^2/2 = 8U_p = 10\omega_0$, is much larger than the photon energy. Depending on the incident particle energy, typical energy spectra extend up to $20-100$ photon orders for these parameters.

The calculations are performed in the Kramers-Henneberger (KH) coordinate frame, whose origin is displaced with respect to the laboratory frame by the quiver amplitude,

$$\xi(t) = \xi_0 \sin(\omega_0 t), \qquad \xi_0 = \mathcal{E}_0/\omega_0^2. \tag{3}$$

The TDSE has the well-known form

$$i\partial_t \psi(x,t) = \left[-\frac{1}{2}\partial_x^2 + V(x+\xi)\right]\psi(x,t). \tag{4}$$

The time-dependent scattering problem has been studied by the method of wavepacket scattering. In the initial state, a wavepacket is launched from the left asymptotic region toward the scattering center. Its time-evolution is followed for 16 laser periods up to a final state with well separated transmitted and reflected wavepackets. Subsequently the energy spectra of the transmitted and reflected wavepackets are analyzed in the asymptotic regions by taking spatial Fourier-transforms of the wavefunction. The initial wavepacket is chosen as a plane wave with a Gaussian envelope,

$$\psi_0(x) = \mathrm{e}^{ik_0 x}\mathrm{e}^{-(x-x_0)^2/d^2}. \tag{5}$$

For initial velocities k_0 in the range between 1 and 5, the initial position x_0 and the width d are chosen as

$$x_0 = -\frac{1}{2}k_0\tau, \qquad \tau = 16\,\frac{2\pi}{\omega_0}, \qquad d = \frac{2}{5}|x_0|. \tag{6}$$

Within the computation time τ, a free wavepacket moves the distance $2|x_0|$ from $-|x_0|$ to $+|x_0|$. Specifically, $\tau \approx 500$, $|x_0| \approx 250$ and $d \approx 100$ for $k_0 = 1$.

III. SCATTERING FROM SINGLE IONS

In this section, we consider scattering from a single ion and discuss the dependence of the energy spectrum on the initial energy of the electrons. To demonstrate the relationship between scattering and ionization, we first choose the initial state

$$\psi_0 = 1. \tag{7}$$

It corresponds to a wavepacket with zero velocity $k_0 = 0$ and infinite width $d \to \infty$. These conditions are similar to those in ATI. In the absence of a preferred drift motion, the effective impact velocity of the electron is determined by the quiver motion in the laser field and by the attractive potential. The calculated energy spectrum is shown in Fig. 1. One actually can recognize the familiar structure of the ATI-plateau. The peaks are separated by the photon energy. Higher photon orders form the scattering plateau extending up to the ATI cut-off,

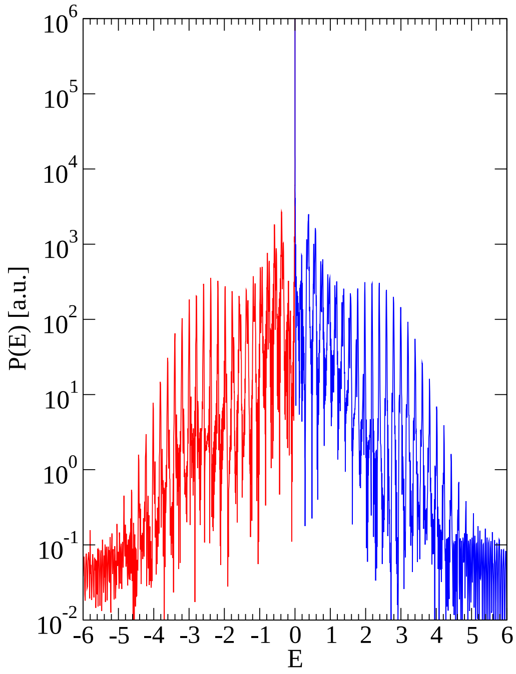

FIG. 1: Energy spectrum for scattering with zero initial momentum. One can observe spatially symmetric ATI-type scattering plateaus on both sides of the scattering center.

$$E_c = 10U_p = 2.5\ . \tag{8}$$

The figure shows both the spectrum on the left and on the right side of the scattering center, being represented by negative and positive energies, respectively. There is nearly perfect spatial symmetry in this case.

We now discuss the scattering of Gaussian wavepackets for a sequence of initial momenta. Increasing the initial momentum k_0, the spatial symmetry is broken and one observes completely different spectra for the transmitted and the reflected wavepackets as shown in Fig. 2. On the right, the scattering plateau disappears and instead an elastic peak with an exponential distribution of sidebands is observed. This corresponds to the fact, that reflection into the right half-space becomes strongly suppressed. It is only possible if an electron, which has already been transmitted is returned to the ion and then is rescattered again. In contrast, the incident electron can be directly

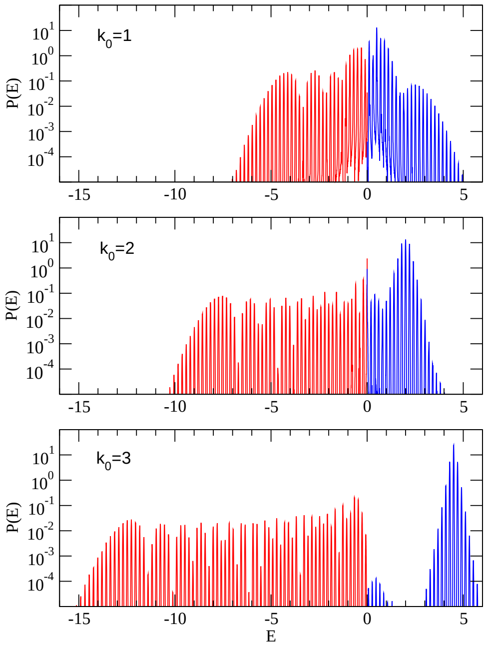

FIG. 2: Energy spectra for scattering with initial velocities velocities $k_0 \geq 1$. With increasing velocities the spectrum becomes spatially asymmetric. The transmitted wavepacket has an exponential energy distribution around the elastic peak. The reflected wavepacket shows a plateau in a broad range of energies.

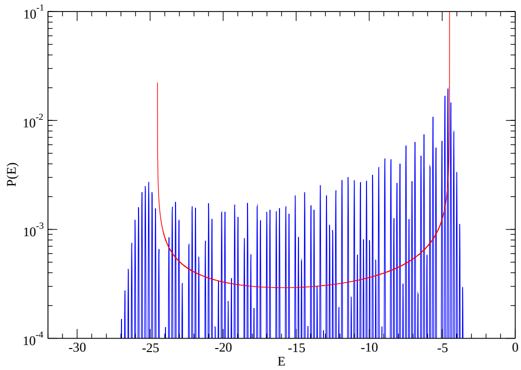

FIG. 3: Energy spectrum for $k_0 = 5$. Comparison of wavepacket scattering with the instantaneous collision model. The average height of the plateau and its cut-offs are well reproduced by the model.

reflected into the left half-space leading to a plateau on this side. Due to the increased initial velocity the plateau gets strongly broadended and fast electrons far above the ATI-cutoff (8) can be generated.

Electron-ion collisions in strong laser fields can be treated by the model of classical instantaneous collisions. For instantaneous elastic collisions at time t_c, the laser field can be taken as constant. From energy conservation, the momentum of the reflected particle is found to be

$$k + p_{\mathcal{E}} = -(k_0 + p_{\mathcal{E}}), \tag{9}$$

where $k_0 > 0$ denotes the drift momentum before and k after the collision and $p_{\mathcal{E}} = v_0 \cos\phi$ the quiver momentum evaluated at the phase $\phi = \omega_0 t_c$. The new drift momentum $k = -(k_0 + 2p_{\mathcal{E}})$ varies between the values,

$$k_1 = -k_0 - 2v_0, \qquad k_2 = -k_0 + 2v_0. \tag{10}$$

The electron will leave the field with an energy

$$E(\phi) = \frac{1}{2}(k_0 + 2p_{\mathcal{E}}(\phi))^2 \tag{11}$$

that depends on the collision phase ϕ. Assuming that the collision phases are randomly distributed within the interval $[0, \pi]$ and that a fraction R of particles is reflected in each collision, the energy distribution can be obtained as

$$P(E) = \frac{R}{\pi}\,\frac{d\phi}{dE} = \frac{R}{\pi|k|\sqrt{(k-k_1)(k_2-k)}}, \tag{12}$$

where k is viewed as a function of $E = \frac{1}{2}k^2$. Corresponding to the momenta $k_{1,2}$, the energy distribution has cut-offs at,

$$E_{1,2} = \frac{1}{2}(k_0 \pm 2v_0)^2. \tag{13}$$

In Fig. 3, the model distribution (12) is compared with a calculated energy spectrum. The model gives an excellent approximation to the averaged quantum distribution with the proper cut-offs. The only unknown parameter in (12) is the reflection coefficient R. For most cases of interest, it can be gained with good accuracy from the field-free scattering problem.

IV. SCATTERING FROM ION-PAIRS

In this section we discuss the formation of a double-plateau distribution in electron collisions with a pair of

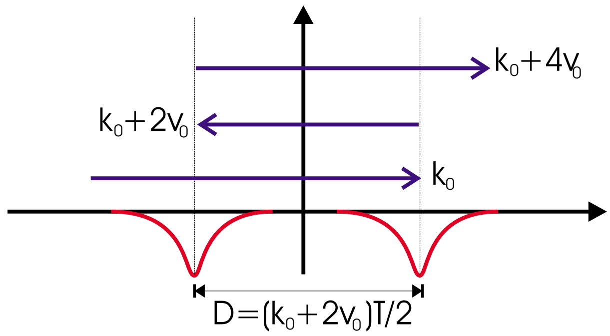

FIG. 4: Double collisions with an ion pair. In each collision, the maximum momentum gain is $2v_0$ if both collisions take place at subsequent maxima of the quiver velocity. The corresponding ion distance D is given by (16).

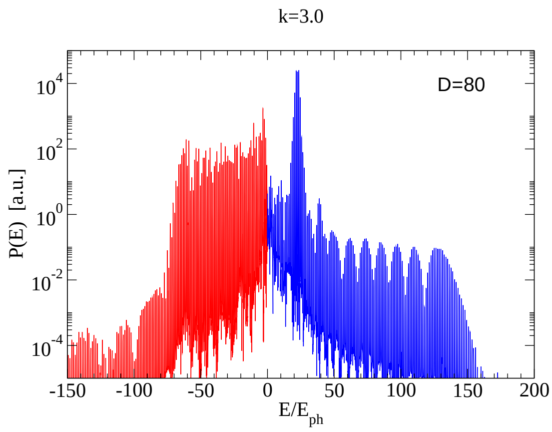

FIG. 5: Double-plateau for scattering at an ion pair. Single-scattering leads to the plateau at the left ($E < 0$), double-scattering to the plateau at the right ($E > 0$). On the right side, one can also recognize the elastic peak of the transmitted wave. The parameters are $k_0 = 3$, $v_0 = 1$, $\omega_0 = 0.2$, $D = 80$, $\epsilon = 0.1$ and $Z = 1$. The energy is represented in units of the photon energy $E_{ph} = \omega$.

ions. At first glance, one might expect the possibility that an electron could collide two times with the same ion. However, such double-collisions will be extremely unlikely since the electron escapes after the first collision. To obtain double-collisions, we therefore consider successive collisions with different ions. The basic requirements for successive collisions with maximum energy gain can be obtained from a classical analysis as shown schematically in Fig. 4. Assume that the electron is launched with velocity k_0 along the x-direction and collides with the right ion with the maximum effective impact velocity $p_0 = k_0 + v_0$ at $t = 0$. Then its velocity will change according to

$$v = \pm p_0 + v_0(\cos\omega_0 t - 1), \tag{14}$$

where the upper sign is taken before, the lower one after the collision. The reflected electron moves in the negative x-direction and collides again with the left ion. For maximum energy gain, the second collision has to take place after one half-period, $\omega_0 t = \pi$, when the velocity reaches its maximum value $p_1 = -k_0 - 3v_0$. At the second collision the velocity change is analogously given by

$$v = \pm p_1 + v_0(\cos\omega_0 t + 1). \tag{15}$$

The average velocity is $\bar{v}_1 = -k_0 - 2v_0$ after the first and $\bar{v}_2 = k_0 + 4v_0$ after the second collision. These are also the velocities in the KH frame. Consequently, one expects two energy plateaus, one on the left side with cut-off $(k_0 + 2v_0)^2/2$ and one on the right side with cut-off $(k_0 + 4v_0)^2/2$. In order to obtain the maximum possible energy gain, the distance between the ions has to be equal to the propagation distance of the electron in the half-period between the two collisions,

$$D = (k_0 + 2v_0)T/2, \qquad T = 2\pi/\omega_0. \tag{16}$$

We have calculated the scattering of a wavepacket by an ion-pair in the framework of the 1d-TDSE. The ions, separated by a distance D, are represented by the potential

$$V = -\frac{Z}{\sqrt{(x+D/2)^2+\epsilon^2}} - \frac{Z}{\sqrt{(x-D/2)^2+\epsilon^2}}. \tag{17}$$

As an example, choosing the parameters $k_0 = 3$, $v_0 = 1$, $\omega_0 = 0.2$, one obtains from (16) the distance $D = 78.5$. The energy spectrum calculated with $D = 80$ shows the expected double-plateau distribution (Fig. 5). The first plateau on the left results from single collisions, the second plateau on the right from double collisions. The height of the first plateau is proportional to the refectivity R, the second one is proportional to R^2. For a single potential without laser field the reflectivity is of the order of a few percent. Specifically, $R \approx 0.04$ for $\epsilon = 0.1$, $Z = 1$ and $k_0 = 3$. The energy cut-offs are in close agreement with the classical estimates,

$$E_1 = \frac{1}{2}(k_0 + 2v_0)^2 = 62.5\omega_0,$$
$$E_2 = \frac{1}{2}(k_0 + 4v_0)^2 = 122.5\omega_0.$$

The maximum energy of the second plateau is sensitive to the distance between the ions. Energy spectra for

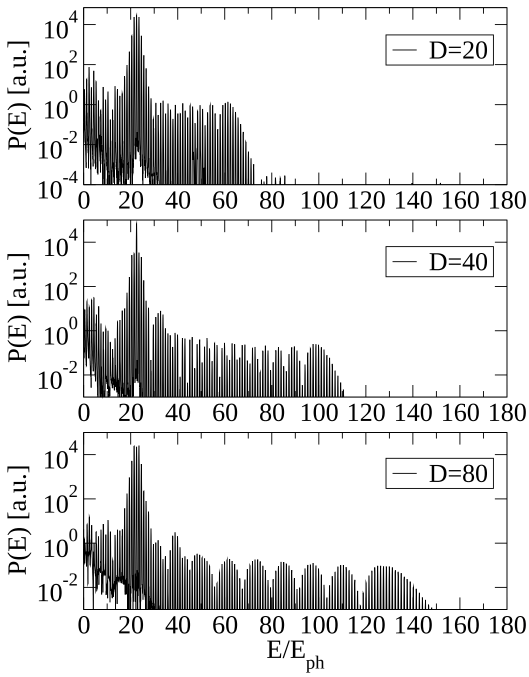

FIG. 6: Second plateau for different ion distances D. The other parameters are $k_0 = 3$, $v_0 = 1$, $\omega_0 = 0.2$, $\epsilon = 0.1$ and $Z = 1$. The energy is represented in units of the photon energy $E_{ph} = \omega$.

different ion distances are compared in Fig. 6. One can recognize that the maximum cut-off energy is actually reached with the optimum distance $D \approx 80$.

V. CONCLUSIONS

In this work, the energy distribution of electrons generated by electron-ion collisions in a strong laser field has been investigated in the framework of the TDSE for a 1d softcore Coulomb-potential. For small initial velocities symmetric ATI spectra with a cut-off at $10U_p$ on both sides of the potential can be reproduced. For larger initial velocities, the energy distribution separates into two parts: The transmitted waves show an exponential distribution about the elastic peak at $k_0^2/2$, the reflected waves a plateau with cut-offs at $(k_0 \pm 2v_0)^2/2$. The plateau can be explained in terms of classical instantaneous collisions. This model can also be generalized to 3d-Coulomb-collisions. The energy distribution can be derived analytically in the framework of instantaneous Coulomb collisions. There is a significant fraction of fast electrons produced by Coulomb collisions at small impact parameters which can be of considerable importance for the ionization dynamics in collisional plasmas[18].

We have extended these studies to scattering by ion pairs and observe a double-plateau as a result of double-collisions. The sensitivity of the maximum energy to the ion distance confirms very well the classical rescattering picture. The maximum energy of the second plateau can only be reached if the time between two successive collisions is one half-period of the laser. This correlation has been confirmed by calculations with different ion distances. As a potential application, ATI experiments could be performed with diatomic molecules. With a first laser pulse the molecule could be dissociated into two atoms, drifting apart from each other. With a second stronger pulse, the atoms could then be ionized. For a suitably chosen delay-time between the pulses the corresponding ATI-spectra should show the double plateau. It would be interesting to demonstrate in such experiments the correlation between the maximum energy of the second plateau and the ion distance.

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