

Soft-collision and cusp electrons in longitudinal momentum distributions for single ionization of He and Ne by proton impact

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The position of the maximum in longitudinal electron momentum distributions, for He and Ne single ionization by proton impact, has been studied as a function of projectile velocity using the continuum-distorted-wave-eikonal-initial-state model. At intermediate to high energies the position of the maximum is determined by low-energy electron emission and it can be related to the soft-collision peak. At intermediate to low energies, the position of the maximum depends on the interplay between soft-collision and cusp electrons, which produces a linear dependence of its position as a function of the projectile velocity.
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The single-ionization process in ion-atom collisions constitutes a major challenge to theory. In a quantum-mechanical description it requires basically knowledge of the states of one electron in the presence of two nuclei. The electron can be bound to one nuclei while in the continuum of the other one (initial state), or in a continuum of both (final state). The difficulty arises from the fact that the Schrödinger equation for the three-body problem cannot be solved exactly. It is only in the last ten years that it has been possible to develop theoretical approximations that take into account the long-range behavior of the Coulomb potential in computational efficient codes.

The most detailed information about the dynamics of the single-ionization process can be obtained from the measurement of doubly differential cross sections (DDCS) as a function of the electron angle and energy. This technique, called electron emission spectroscopy (EES), has yielded a huge amount of information by using different projectiles (protons, antiprotons, highly charged ions, etc.) at different impact energies [1]. At high energies, distorted-wave models, such as the continuum-distorted-wave-eikonal-initial-state (CDW-EIS) [2,3], are able to reproduce, with a very high accuracy, the experimental findings [4,5]. At intermediate impact energies such models are only in qualitative agreement with experiments. This is due to the fact that, in this case, these models are in their limit of validity and that most experiments cannot separate the contribution from different processes that lead to an emitted electron (multiple ionization, transfer ionization, etc.).

Recently, there has been a renewed interest in the study of the single- and multiple-ionization processes due to the development of a new experimental technique [cold target recoil-ion momentum spectroscopy (COLTRIMS)] [6], which allows one to obtain information about the dynamics of the process in a different fashion. This technique provides momentum distributions of the emitted electron, the recoil ion, and the projectile, which can be studied in coincidence. If the electron spectra are taken without any information

about the recoil ion or the projectile, it is called electron emission momentum spectroscopy (EEMS). One of the main features of this technique is that it allows one to study, with great accuracy, details of the spectra of emitted electrons, which are difficult to study with EES. A good example of this feature is the recent measurement of ultra-low-energy electrons in the single ionization of He by highly charged ion impact [7].

It is obvious that measurements from EES and EEMS give different views of the same processes. Therefore, what is well known from EES can be used to understand the new results from EEMS. Such is the case of the longitudinal electron momentum distributions for proton impact on He and Ne measured with EEMS at intermediate projectile velocities (\vec{v}_p) [8,9]. These measurements show two main features: a large maximum at longitudinal electron velocities (v_{ez}) between that of the soft-collision peak ($v_{ez} \approx 0$) and the cusp ($v_{ez} \approx v_p$) and, at some impact velocities, a hump at $v_{ez} = v_p$. Theoretical models, such as CDW-EIS or simulations with the classical trajectory Monte Carlo (CTMC), give similar results that are in close agreement with experiments. While the second feature can be attributed to the presence of the cusp, there are no simple models to explain the position of the maximum. From EES measurements it is well known that the electrons are emitted mostly with low energies, showing in the DDCS the characteristic soft-collision peak. Therefore it has been suggested that the mechanism that determines the position of the maximum (v_{ez}^M) is that of saddle-point electron emission [10], where the emitted electron is stranded on the saddle point produced by the projectile and residual target Coulomb potentials. This mechanism was introduced previously to explain certain results obtained with EES [11], and since then it has been a subject of controversy (see [12,13], and references therein). It predicts that v_{ez}^M is proportional to the projectile velocity. However, calculations with CDW-EIS and CTMC show that, on the contrary, from intermediate to high velocities v_{ez}^M decreases with increasing v_p [14,15], in qualitative agreement with experiments [8]. At high impact velocities the electron is emitted mainly from collisions at large impact parameters in dipolar transitions. This process produces a characteristic distribution that maxi-

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mizes in the perpendicular direction; therefore $v_{ez}^M \rightarrow 0$ as the projectile velocity increases. From low to intermediate velocities CDW-EIS and CTMC predict that v_{ez}^M increases with v_p , in apparent agreement with the saddle-point mechanism. It is clear that to explain this behavior it is necessary to understand, in the first place, why the maximum appears in a certain position. The answer to this question will explain the dependence on the projectile velocity.

In the present work we analyze doubly differential cross sections as a function of the longitudinal and one of the perpendicular components of the electron momentum using the CDW-EIS model. The results show that the position of the maximum can be related to the behavior, as a function of the projectile velocity of the soft-collision peak and the cusp observed in measurements with EES.

As a first step it is important to understand the physical meaning of the longitudinal momentum distributions. In fact, they can be readily identified as singly differential cross sections (SDCS) as a function of the longitudinal electron momentum. This cross section depends on just one component of the electron momentum and is obtained from an integration over the other components (v_{ex}, v_{ey}); therefore some information about the dynamics is lost. The longitudinal momentum distribution for a given value of v_{ez} represents the probability for emission at that value of the longitudinal momentum, while the other components take any value. Therefore the longitudinal momentum distribution is not a measure of the cross section in the forward direction. This information is given by a doubly differential cross section where the momentum in the perpendicular direction is taken equal to zero. This information is buried in the longitudinal momentum distribution due to the integration mentioned above and there is no direct functional relation between them. For this reason the saddle-point mechanism, which can only appear at the forward direction, is not able to predict the position of the maximum and its dependence on the projectile velocity.

To explain this behavior we need more detailed information about the process, which we obtain from the doubly differential cross sections as a function of v_{ey} and v_{ez} . These DDCS are obtained from the integration over the remaining transverse component (v_{ex}). Note that the transverse components v_{ex} and v_{ey} are equivalent, due to the cylindrical symmetry of the collision. To study the contribution from the different values of v_{ey} , we define a reduced longitudinal electron momentum distribution as

$$\frac{d\sigma^*}{dv_{ez}} = \int_{-v_{ey}^*}^{+v_{ey}^*} dv_{ey} \frac{d^2\sigma}{dv_{ey} dv_{ez}}. \quad (1)$$

When $v_{ey}^* = 0$ the reduced cross section corresponds to the doubly differential cross section. As it increases the reduced cross section takes into account an increasing amount of emission in the y direction. Finally, when $v_{ey}^* \rightarrow \infty$ we retrieve the longitudinal electron momentum distribution as measured in the experiments.

In Figs. 1–3 the reduced cross sections are presented for single ionization of helium by proton impact at the projectile velocities used in [9] ($v_p = 2.39, 1.63,$ and 1.15 a.u., respectively). The four curves in each figure correspond to $v_{ey}^* = 0.1, 0.2, 0.5$ a.u., and ∞ . When $v_{ey}^* = 0.5$ a.u. the reduced

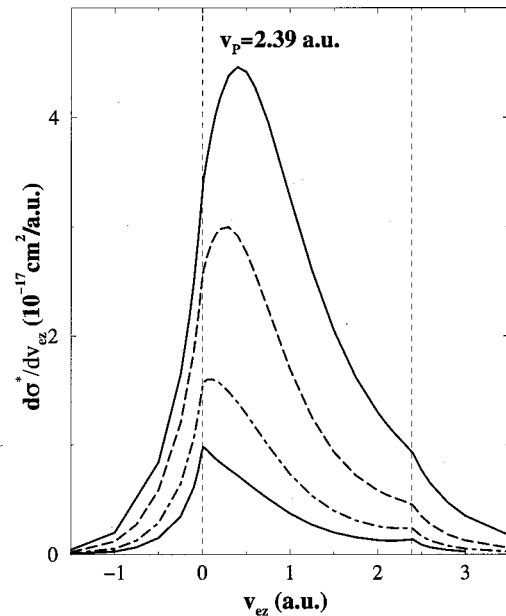


FIG. 1. Reduced cross section as a function of the longitudinal electron velocity for 2.39 a.u. proton impact on He. Present CDW-EIS results: solid line, lower curve, $v_{ey}^* = 0.1$ a.u.; dot-dashed line, $v_{ey}^* = 0.2$ a.u.; dashed line, $v_{ey}^* = 0.5$ a.u.; solid line, upper curve, $v_{ey}^* \rightarrow \infty$. Vertical short-dashed lines correspond to $v_{ez} = 0$ and $v_{ez} = v_p$.

cross section already resembles the longitudinal momentum distribution, showing the same qualitative behavior. Thus, as expected from what is known from EES, the main variations of the cross sections occur at small transverse momenta (small emission angles). At the highest impact velocity (Fig. 1) and for $v_{ey}^* = 0.1$ a.u. the reduced cross section is quite similar to a DDCS from EES in the forward direction with a well-separated soft-collision peak from the cusp. Neither of the peaks diverge, due to the integration over v_{ex} , which

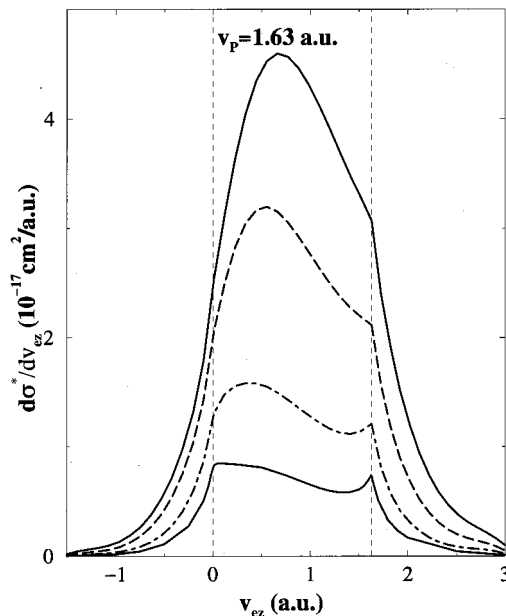


FIG. 2. Same as Fig. 1 but for 1.63 a.u. proton impact on He.

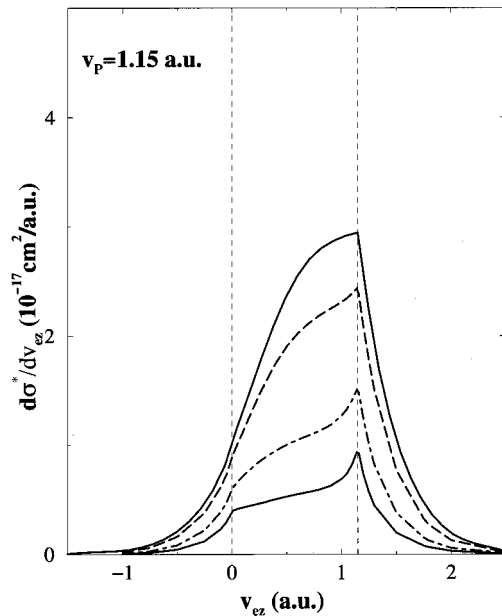


FIG. 3. Same as Fig. 1 but for 1.15 a.u. proton impact on He.

produces an effect similar to that of the integration over the acceptance angle in EES measurements of the cusp. As v_{ey}^* increases, the relative intensity of the cusp decreases, and when $v_{ey}^* \rightarrow \infty$ it only remains as a hump or as a change in the slope of the distribution. However, the soft-collision peak presents a different behavior: as v_{ey}^* increases the position of the peak shifts and gives rise to the maximum in the longitudinal momentum distribution. As the impact velocity decreases (Fig. 2) the main difference is that for $v_{ey}^* = 0.1$ a.u. the position of the cusp begins to overlap with the broad soft-collision peak. This effect is much more pronounced at the lowest impact velocity (Fig. 3). As v_{ey}^* increases, the overlap between the peaks defines the shape of the longitudinal momentum distribution. In this case the maximum is positioned not on the shifted soft-collision peak but on the cusp. As a consequence, as the impact velocity is further decreased, the maximum of the longitudinal momentum distribution follows the position of the cusp, which is located at the projectile velocity. When the peaks separate, the position of the maximum depends on the soft-collision peak because, as is well known, the relative intensity of the cusp is much smaller. Therefore it is the interplay between the peaks that can explain the dependence of v_{ez}^M on v_p and not the saddle-point mechanism.

From the previous discussion it is clear that from intermediate to low velocities the position of the maximum depends on the contribution from electrons emitted with velocities ranging from the soft-collision peak to the cusp. As the velocity increases, the contribution from the latter diminishes and the maximum can be related to the emission of low-energy electrons. However, this is not enough to explain why the maximum is still shifted from the soft-collision peak. To understand this behavior we consider the emission from a different target (Ne). The projectile velocity corresponds to that of Fig. 2. The results for Ne [Fig. 4(b)] are on the whole quite similar to those for He. The main difference is that the shift of the maximum is smaller and that this is due to the fact, which can be seen more clearly in the case v_{ey}^*

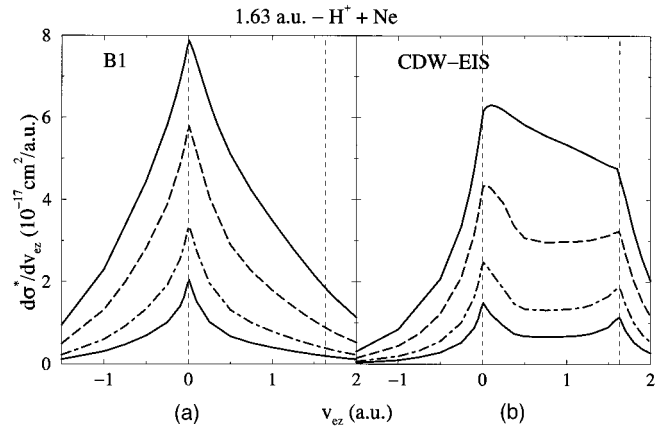


FIG. 4. Reduced cross section as a function of the longitudinal electron velocity for 1.63 a.u. proton impact on Ne.

$= 0.1$ a.u., that for Ne the cross section for electrons emitted with velocities in between the two peaks is smaller relative to the peaks than in the case of He. As a consequence, the soft-collision peak is more symmetric in the case of Ne. We can thus attribute the shift of the maximum to the well-known forward-backward asymmetry of low-energy electron emission. It has been shown that this effect depends markedly on the target and it is much more important in the case of He than for Ne [16]. Therefore the shift of the maximum is new evidence of the forward-backward asymmetry of the soft-collision peak. This is supported by the results presented in Fig. 4(a) obtained with the first-Born approximation (B1), which, as expected, gives a symmetric distribution. It must be noted that calculation with B1 for He (not shown here) also presents a shift, which is smaller than that given by CDW-EIS. This is in agreement with the fact that the asymmetry has contributions from two sources: the non-Coulomb behavior of the target potential, which is considered in B1, and the two-center effect, which is absent from B1. Therefore the shift obtained from CDW-EIS is always larger than that obtained from B1.

In conclusion, it has been shown that the position of the maximum in longitudinal electron momentum distributions depends markedly on the impact velocity. At intermediate velocities, when the soft-collision peak and the cusp are close, there is an enhanced contribution from the latter that therefore determines the position of the maximum. In this range the position of the maximum is proportional to the projectile velocity. When both peaks separate, as the projectile velocity increases, the position of the soft-collision peak determines the position of the maximum because the relative contribution from cusp electrons is very small. In this range the position of the maximum is determined by the asymmetric emission of low energy electrons. As the projectile velocity increases dipolar emission begins to dominate and the maximum approaches to zero longitudinal electron momentum. Careful experiments in a large range of projectile velocities are needed to study in much more detail the interplay between the soft-collision peak and the cusp.

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