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LETTER TO THE EDITOR

Longitudinal momentum distributions in ionization of helium by fast, highly charged projectiles

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Abstract. The longitudinal momentum distributions for the recoil ion, the electron and the projectile momentum transfer in single ionization of He by 3.6 MeV amu^{-1} Ni^{24+} impact are calculated using the CDW-EIS method within the independent electron approximation. Results are compared with the measurements and CTMC calculations of Moshammer *et al* (1994). It is found that the CDW-EIS theory explains qualitatively the observed enhancement of the electron distribution in the forward direction, and the enhancement of the recoil-ion distribution in the backward direction. Our calculations show discrepancies with the measurement regarding the positions for the maxima of these distributions. A calculated electron energy spectrum is in good agreement with the measurement.

The development of recoil-ion momentum spectroscopy techniques [1–3] in recent years has made it possible to determine the final-state momentum distributions of all the collision products. In a recent experiment, Moshammer *et al* [1] measured the longitudinal electron momentum distribution, the longitudinal recoil-ion momentum distribution, the longitudinal projectile momentum transfer distribution and the differential cross section in electron energy for the single ionization of He atoms by 3.6 MeV amu^{-1} Ni^{24+} ions. Theoretical analysis for such detailed experiments involving highly charged ions is not available except at the level of using the classical trajectory Monte Carlo method (CTMC, see [1, 3]) where the motion of the electron is described classically.

In a recent paper [4], we have developed a complete theoretical formulation of the description of longitudinal recoil-ion momentum distribution in ionizing collisions between fast bare ions with atomic targets. In this letter we analysed the results of Moshammer *et al* [1] by the continuum-distorted-wave–eikonal-initial-state approximation (CDW–EIS) to check the validity of this theory. The CDW–EIS method, proposed by Crothers and McCann in 1983 [5] (see the review article by Fainstein *et al* [6] and references therein), has the important feature that the ionized electron sees the Coulomb field from both the target and the projectile ions, and the wavefunction satisfies the correct asymptotic Coulomb boundary conditions. The standard CDW–EIS theory [5], which was developed for studying three-body collision systems, has to be modified to treat ionization of multi-electron targets. Following the work of Fainstein *et al* [6], we used an independent electron model to treat the two-electron helium target. The initial He state is described by the Hartree–Fock wavefunction while the final state is given by the hydrogenic wavefunction with an effective charge. As in any independent electron model, no electron correlation is considered. However, correlation

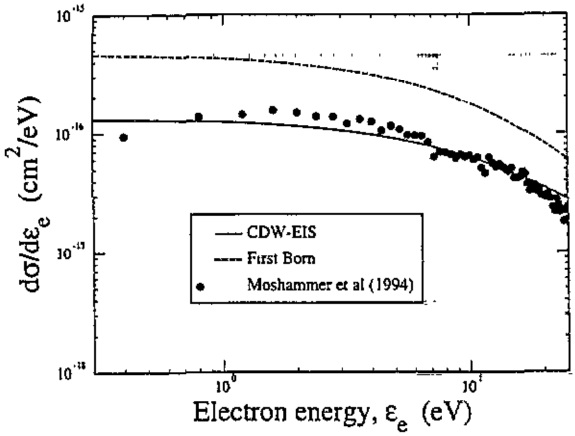

Figure 1. Differential cross section as a function of electron energy for ionization of He by 3.6 MeV amu^{-1} Ni^{24+} ions. Full circles: experimental data from Moshammer *et al* [1]; full curve: present CDW-EIS calculation; broken curve: present first Born calculation.

effects in single processes (single ionization) are known to be less important than in double processes, such as double ionization.

For comparison, we also performed calculations within the first-order Born theory. For such collisions involving highly charged ions, the first Born approximation is not expected to be valid. By comparing the results from the two calculations, on the other hand, we can identify special features in the experimental spectra which are due to the two-centre effect included in the CDW-EIS theory.

Measurements of energy and angular distributions of the ejected electron have long been regarded as the most important and fruitful approach to exploring ionization dynamics. The experiment of Moshammer *et al* [1] determined the single-ionization cross section differential in the ejected electron energy $(\frac{d\sigma}{d\epsilon_e})$ and found good agreement with the CTMC calculations. We note that there are several normalization errors in the original publication [1]. Corrected data were obtained from the authors. In addition, the experimental data were normalized to the total ionization cross section which should be corrected since only electrons with energies up to 50 eV were measured. To take this into account, we multiplied the experimental data by 0.85, the theoretical percentage obtained from the present CDW-EIS theory. In figure 1 we compare the corrected experimental data with our calculations using the CDW-EIS theory and the first Born approximation. Two effective charges were used for the hydrogenic continuum in the CDW-EIS calculations. The first is $Z = 1.34$, arising from the binding energy of the He atom. The second is the variational charge, $Z = 1.69$. In the latter case, the initial state is also described by a hydrogenic state with the same effective charge. In figure 1, electron energy spectrum obtained from $Z = 1.34$ is shown. Results from $Z = 1.69$ are not shown. They are slightly larger (within 10%) at the energy range between 0.1 and 50 eV. At higher energies, they can differ by 20%. Cross sections obtained from the first Born approximation are a factor of 3 to 4 times larger than the experimental data. The failure of the first Born theory is not unexpected for collisions of He atoms with 3.6 MeV amu^{-1} Ni^{24+} ($v = 12$ au) ions. The Z_p/v (Z_p is the charge of the projectile ion) is larger than 1. In figure 1 we notice that the prediction of the CDW-EIS agrees rather well with the experimental data. At small electron energies, there is a somewhat larger difference between theory and experiment. In particular, experimental data seem to show a maximum around 2 eV whereas the present calculation does not. Berg *et al* reported measurement of absolute total ionization cross section for this system [7]. Our calculated total ionization cross sections for $Z = 1.34$ and $Z = 1.69$ are 2.6×10^{-15} cm^2 and 3.0×10^{-15} cm^2, respectively, in good agreement with their measured value of $2.4 \times 10^{-15} \pm 0.5$ cm^2.

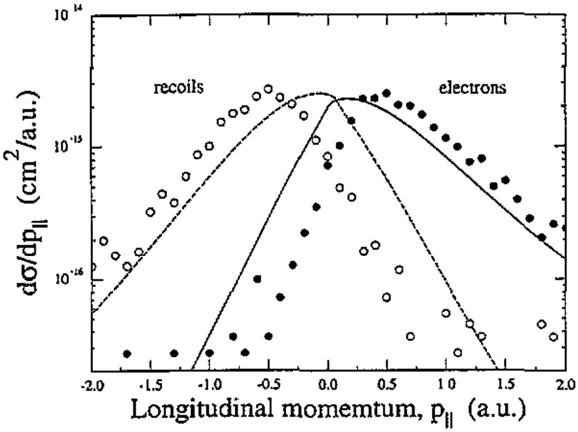

Figure 2. *Calculated longitudinal momentum distributions for the electron (full curve) and the recoil ion (broken curve) in single ionization of He by 3.6 MeV amu^{-1} Ni^{24+} ions. Experimental data are from Moshammer et al [1].*

In ion–atom ionization, it is rather difficult to measure low energy electrons accurately even though they compose the bulk of the total and differential ionization cross sections. The new technique of measuring momentum distributions of product particles provides an alternative approach of studying ionization dynamics. In the experiment of Moshammer *et al* [1], the longitudinal electron momentum distribution $\left(\frac{d\sigma}{dp_{e\|}}\right)$ and the longitudinal recoil-ion momentum distribution $\left(\frac{d\sigma}{dp_{R\|}}\right)$ are measured. They also extracted the longitudinal projectile momentum transfer distribution $\left(\frac{d\sigma}{dp_{P\|}}\right)$. Here $p_{e\|}$, $p_{R\|}$ and $p_{P\|}$ are, respectively, the longitudinal momenta for the electron, the recoil ion and the longitudinal projectile momentum transfer.

In figure 2, we show the longitudinal momentum distributions for the electron (full curve) and the recoil ion (broken curve) calculated using the CDW-EIS theory with effective charge $Z = 1.34$. Also shown are the measurements of Moshammer *et al* [1]. Note that the two distributions are similar where the electron distribution has a peak at a small positive value of longitudinal momentum and most electrons are emitted in the forward direction (i.e. along with the projectile), while the recoil-ion distribution has a peak at a negative value of longitudinal momentum and most are ejected in the backward direction. These two distributions are related through the conservation of momentum of the electron, recoil ion and the projectile. In order to establish the relation, we follow the formulation detailed in our recent paper [4].

The bridge between the conventional measurement of energy and angular distributions of the ejected electron and the momentum distributions of the recoil ion and electron is the conservation of energy and momentum of the three particles. For fast collisions, the longitudinal momentum conservation requires that

$$p_{R\|} = p_{P\|} - p_{e\|} = (\varepsilon_e - \varepsilon_i)/v - k_e \cos\theta_e \tag{1}$$

which is related to the Q value of the collision process ($p_{P\|} = Q/v$). The second identity in (1) is valid to the order of the ratio of the electron mass with respect to the projectile mass. Here k_e is the momentum of the ionized electron, θ_e is the electron emission angle with respect to the incident beam direction, and ε_i is the ionization energy of the initial target He atom ($\varepsilon_i = -0.903$ au). By means of (1), we can obtain longitudinal momentum distributions from the T-matrix or the DDCS. For a given $p_{e\|}$, the longitudinal electron momentum distribution can be obtained by integrating the DDCS over electron energy,

$$\frac{d\sigma}{dp_{e\|}} = \int_{p_{e\|}^2/2}^{\infty} \frac{1}{k_e} \frac{d^2\sigma}{d\varepsilon_e\, d(\cos\theta_e)} d\varepsilon_e . \tag{2}$$

For a given $p_{R\|}$, the longitudinal recoil-ion momentum distribution can also be obtained by integrating the DDCS,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}p_{R\|}} = \int_{\varepsilon_e^-}^{\varepsilon_e^+} \frac{1}{k_e} \frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon_e\,\mathrm{d}(\cos\theta_e)}\mathrm{d}\varepsilon_e \tag{3}$$

but the lower and upper integration limits are implicitly specified by the longitudinal momentum conservation (1). For the three-body system, it can be shown that the longitudinal momentum of the ionized electron is given by [4]

$$k_e^{\pm}(\theta_e) = v\cos\theta_e \pm \sqrt{v^2\cos^2\theta_e + 2(p_{R\|}v - |\varepsilon_i|)} \tag{4}$$

and $\varepsilon_e^{\pm} = \frac{1}{2}(k_e^{\pm})^2$.

We now return to figure 2. Let us first analyse the longitudinal electron momentum distribution as given by (2). It is obvious that soft electrons should contribute more to the longitudinal momentum distribution since they are the dominant component in the DDCS. The broad peak of the longitudinal electron momentum distribution is due to the soft electron peak in the DDCS as $k_e \to 0$. To understand the enhancement of soft electron emission in the forward direction, we follow the conventional parametrization of the DDCS (see Suarez *et al* 1993 [8]),

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon_e\,\mathrm{d}(\cos\theta_e)} = [\beta_0(\varepsilon_e) + \beta_1(\varepsilon_e)P_1(\cos\theta_e) + \beta_2(\varepsilon_e)P_2(\cos\theta_e)] \tag{5}$$

where $P_l(\cos\theta_e)$ is the lth-order Legendre polynomial. If $\beta_1 = 0$, the DDCS for the soft electrons is isotropic. If $\beta_1 > 0$, the forward electrons are enhanced. This well known effect in the DDCS causes the shift and enhancement of forward electrons in the longitudinal momentum distribution observed in figure 2. Compared with experiment, there is a notable difference regarding the position of the peak. The CDW-EIS theory predicts the peak at $p_{e\|} = 0.17$ au, which is smaller than the experimental shift of 0.5 au. We did further calculations using the effective charge $Z = 1.69$. The shape and the position of the maximum in the momentum distribution do not change. However, the magnitude is about 10% larger on the left-hand side of the peak and 20% larger on the right-hand side of the peak. This is consistent with our earlier discussion on the electron energy spectrum using the two effective charges. Thus the disagreement between the present CDW-EIS theory and the experiment appears unmodified with the change of target screening. Except for this overall shift relative to the experiment, the shape of the distribution and the enhancement of the forward electrons are well represented by the present CDW-EIS calculations. It should also be mentioned that the maximum location from CTMC calculations are in agreement with the experiment [1], besides the normalization requirement.

Next we consider the longitudinal recoil-ion momentum distribution as given by (3). The shape of the distribution is similar to that of the electron. In figure 2, the longitudinal recoil-ion momentum distribution (obtained with $Z = 1.34$) is mostly in the backward direction. This aspect is a direct consequence of momentum balance between the electron and the recoil ion. However, the projectile also carries away some momentum (see next paragraph) so that the electron and recoil ion peaks are not symmetric. The peak of the recoil-ion momentum distribution can be predicted in our theory. Consider (3)–(5) the longitudinal recoil-ion momentum for soft electron with zero velocity is given by $p_{R\|}^s = |\varepsilon_i|/v$, which is about 0.075 au. If the soft electron distribution is isotropic in the DDCS, the longitudinal recoil-ion momentum distribution should be peaked at 0.075 au. However, the enhancement of soft electrons emitted in the forward direction results in an enhancement of recoiling ions in the backward direction. In our calculations, the peak of the longitudinal recoil-ion

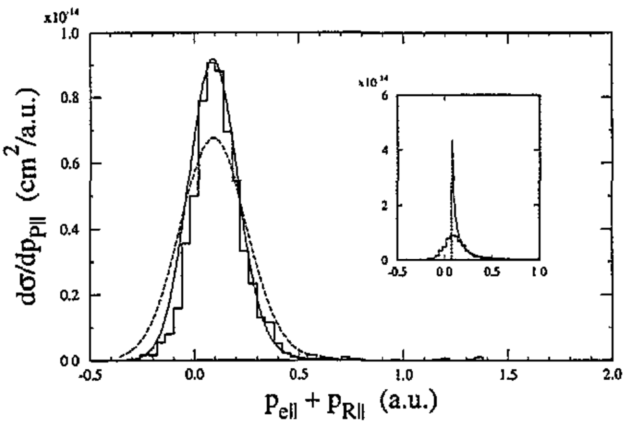

Figure 3. Calculated longitudinal projectile momentum transfer distribution in single ionization of He by 3.6 MeV amu^{-1} Ni^{24+} ions convoluted to a Gaussian distribution. Full curve: for Gaussian width of 0.16 au; broken curve: for Gaussian width of 0.22 au. Experimental data are from Moshammer *et al* [1]. The inset shows the calculated longitudinal projectile momentum transfer distribution without convolution.

momentum distribution is shifted to a lower value at −0.08 au which is to be compared with the experimental value of −0.5 au. As in the electron distribution, we also have a large difference between the theory and experiment on the position of the recoil-ion distribution. Again, this difference can not be explained by changing the target screening charge.

From the figure 2 of Moshammer *et al* [1], one can extract the longitudinal projectile momentum transfer distribution $\frac{d\sigma}{dp_{P\parallel}}$. The overall longitudinal projectile momentum transfer provides a measure of the inelasticity of the collision process. In light of the momentum and energy balance (1), it is straightforward to obtain

$$\frac{d\sigma}{dp_{P\parallel}} = v\frac{d\sigma}{d\varepsilon_e}\,. \tag{6}$$

In figure 3, we compare the calculated (obtained with $Z = 1.34$) and measured longitudinal projectile momentum transfer distribution. According to (1) and (6), the theoretical longitudinal projectile momentum transfer distribution starts as a sharp peak at $p_{P\parallel} = |\varepsilon_i|/v = 0.075$ au, corresponding to zero-energy electron emission, and decreases rapidly to zero as $p_{P\parallel}$ increases. To compare with experiment, we convolute our theoretical result by means of a Gaussian distribution representing the experimental resolution. Consider two widths of the Gaussian distribution. One is 0.16 au (full curve) and the other is 0.22 au (broken curve), the latter being the half-width of the experiment. The agreement between theory and experiment is excellent for Gaussian convolution with a width of 0.16 au

We have also performed calculations for longitudinal electron and recoil-ion momentum distributions with the first Born theory. The results are much larger than the experiment. In addition, at high velocity, the longitudinal electron momentum distribution is peaked at $p_{e\parallel} = 0$ au and the longitudinal recoil-ion momentum distribution is peaked at $p_{R\parallel} = |\varepsilon_i|/v = 0.075$ au, independent on the projectile charge. The shift in the peak positions observed in the experiment is due to the post-collision interaction between the outgoing projectile and the electron. Such interaction is accounted for with the CDW-EIS theory but not in the first Born theory.

In conclusion, we have performed a quantum mechanical analysis of the longitudinal momentum distribution for all three particles including the projectile, target recoil ion and electron, in the ionization of He atoms by fast, highly charged Ni^{24+} ions. The main features of the measurement are explained by the current CDW-EIS theory within the independent electron approximation. The calculated electron energy spectrum and longitudinal projectile momentum transfer distribution are in good agreement with the experiment. The calculated longitudinal recoil-ion and electron momentum distributions show enhancements due to the preference of emission of soft electrons in the forward direction. While the CDW-EIS theory correctly predicts the enhancements and the peaks in the longitudinal momentum distributions for both recoil ions and electrons, there is an apparent overall shift in the momentum distributions in comparison with experiment. Further investigations in both theory and experiment are needed to resolve this discrepancy. We have also shown that the first-order Born theory fails to explain the observed phenomena.

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References

[1] Moshammer R *et al* 1994 *Phys. Rev. Lett.* **73** 3371
[2] Wu W *et al* 1994 *Phys. Rev. Lett.* **72** 3170
[3] Dörner R, Mergel V, Zhaoyuan L, Ullrich J, Spielberger L, Olson R E and Schmidt-Böcking H 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 435
[4] Rodriguez V D, Wang Y D and Lin C D 1995 *Phys. Rev.* A accepted for publication
[5] Crothers D S F and McCann J F 1983 *J. Phys. B: At. Mol. Phys.* **16** 3229
[6] Fainstein P D, Ponce V H and Rivarola R D 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 3091
[7] Berg H *et al* 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 3655
[8] Suárez S, Garibotti C, Meckbach W and Bernardi G 1993 *Phys. Rev. Lett.* **70** 418