Out-of-plane \((e,2e)\) experiments on helium
L = 0, 1, 2 autoionizing levels

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Abstract. We present out-of-plane \((e,2e)\) measurements (using an incident electron energy of 488 eV) and calculations for the helium L = 0, 1, and 2 autoionizing levels and for direct ionization [1]. While the recoil peak almost vanishes in the angular distribution for direct ionization, it remains significant for the autoionizing levels and exhibits a characteristic shape for each orbital angular momentum \(L = 0, 1, 2\). These findings can qualitatively be explained by an \(L\)-dependent addition to the ionization amplitude, but only a second-order model in the projectile–target interaction can quantitatively reproduce the observed magnitudes of the recoil peaks. We present the data as both angular distributions and energy spectra for the resonances. Preliminary experimental out-of-plane \((e,2e)\) (using incident electron of 150 eV) results will also be shown. The experimental part of this work is being carried out using an existing \((e,2e)\) apparatus modified to allow the electron gun (see figure 2) to move on the surface of a (mathematical) cone [2]. This permits the measurement of out-of-plane \((e,2e)\) angular distributions, for a full 360°, using a special geometry that allows out-of-plane conditions to be combined with the binary peak in a single measurement [2].

1. Introduction
By the dawning of this millennium it appeared that theory could accurately describe charged-particle scattering from helium atoms (at least for relatively high incident particle energies). An example of such a scattering process is the direct ionization of helium by charged particle impact with incident momentum \(\vec{k}_0\); a 3D cartoon of a representative Plane Wave Born Approximation (PWBA) calculation for such a process is shown in figure 1. The scattered electron trajectory is labelled in the figure as \(\vec{k}_{sc}\) and the ejected electron intensity in a particular direction is proportional to the position vector to the surface in that direction. The angular distribution of the ejected electrons is rotationally symmetric around the momentum transfer \(\vec{K} = \vec{k}_0 - \vec{k}_{sc}\), with a large binary peak in the +\(\vec{K}\) direction, and a much smaller recoil peak in the −\(\vec{K}\) direction (typically for \(K > \sim 0.7\) au). In the figure, plane I is the scattering plane (and corresponds to a coplanar experiment), and plane II is perpendicular to \(\vec{K}\) and the scattering plane.

Despite great advances in the understanding of scattering processes, there have been several kinematically complete experiments conducted over the past several years incorporating an out-of-plane geometry and involving charged particle impact ionization of a variety of atomic targets that were not well described by theory. A significant example of this was the work published by Schulz, et al. [3] which involved He ionization by fast C\(^{6+}\) ions. In that experiment, the angular
distribution of electrons ejected into plane I (as defined in figure 1) agreed well with theory, but the experimental results in plane II disagreed with expectations by a factor of between three and five; no calculations to date have been able to satisfactorily reproduce these data [1]. Somewhat smaller discrepancies were found in an \((e,2e)\) experiment carried out with equivalent kinematics [4]. Out-of-plane experiments on Mg [5, 19] found dramatic deviations from the rotational symmetry about \(\vec{K}\). Such discrepancies continue to provide ample motivation for further experimental studies.

Figure 1. Representative PWBA calculation of an ejected electron angular distribution for direct ionization. See text for details.

These experiments on He direct ionization are examples of three-body kinematics because the 1s electron common to the initial state and the residual ion is essentially a spectator [18]. Helium ionization—excitation on the other hand, where the ion is left in an excited state, is a four-body process and hence presents a much greater challenge to theory; coplanar experiments have recently investigated this process [16, 17, 18]. It was found that second-order models in the projectile—target interaction were essential to get good agreement when the two outgoing electrons had differing energies. However, even these theories did not do so well for the case of symmetric energy sharing [27].

We have performed out-of-plane experiments (spanning plane III of figure 1) on autoionizing levels, namely the three singlet He levels \((2s^2)^1S, (2p^2)^1D,\) and \((2s2p)^1P\) (see table 1). This process may be written as

\[
\text{He}(1s^2) + e_0 \rightarrow \text{He}^+(1s) + e_{sc} + e_{ej}.
\]

(1)

Since He autoionization by electron impact involves both direct ionization and the excitation of doubly excited resonances, it is an example of mixed three-body and four-body processes. Note that our experiments were carried out in a kinematic regime \((K \approx 2)\) for which the \(C^{6+}\) data on direct ionization [28] showed no out-of-plane deviation from theoretical expectations, \(i.e.,\) the data points at 90° to the scattering plane (the intersection of planes II and III in Fig. 1) were less than 2% of the binary peak. Our experiments therefore test how well theory can describe out-of-plane four-body kinematics.
Table 1. Helium autoionizing levels and relevant parameters obtained from the literature [13, 14, 15]. The energy above the ground state is $E_L$, where $L$ is the orbital angular momentum of the level, $E_{ej}$ is the corresponding ejected electron energy, and $\Gamma_L$ is the level width.

| $E_L$(eV) | $E_{ej}$(eV) | $\Gamma_L$(meV) |
|-----------|--------------|-----------------|
| $2s^2\,^1S_0$ | 57.84 | 33.25 | 120 |
| $2p^2\,^1D_2$ | 59.91 | 35.32 | 57 |
| $2s2p\,^1P_1$ | 60.15 | 35.56 | 38 |

2. Modified (e,e) apparatus

There are a number of (e,e) spectrometers in existence designed for out-of-plane measurements: multidetector systems using fixed spherical [6] or toroidal [7] sector energy analyzers, systems where all components can move [8], and the “reaction microscope” which can collect data over almost $4\pi$ solid angle [9]. All of these were purpose built for out-of-plane measurements. The apparatus used for our experiments was originally designed and constructed to perform coplanar experiments (as described previously in [10, 11]) and has been modified for out-of-plane operation; see [2] for a detailed description of these modifications.

Of interest here are the following components of the apparatus:

(i) An unmonochromated electron gun mounted such that it, and therefore the incident electron direction $\hat{k}_0$, can be moved about on what amounts to the surface of a cone; the geometry of this arrangement is shown in figure 2, while figure 3 shows the physical implementation.

(ii) A gas beam that effuses from a nozzle that is attached to the same mount as the electron gun – ensuring that the position of the atomic beam with respect to the electron beam is fixed.

(iii) Two ejected electron detectors, mounted opposite each other on a single turntable that can rotate in the $xz$-plane as shown.

(iv) A scattered electron detector mounted on a turntable in the $xz$-plane that is coplanar with, but can move independently of, the turntable for the ejected electron detectors.

During an experiment, the scattered electron detector is fixed so that its entrance optics are coaxial with the axis of the electron gun mount. Movement of the electron gun results in rotation of the scattering plane, while scattering angle remains constant. For the experiments reported here, the ejected electron detectors are positioned so that the detected ejected electron trajectories are perpendicular to the scattered direction (fig 1 Plane III).

3. Results

We carried out (e,e) out-of-plane experiments for the special kinematical case where the momentum transfer vector is perpendicular to the scattered electron direction. The condition for this is $\theta_{sc} = \arcsin \left( \sqrt{\Delta E/E_0} \right)$, where $\Delta E$ is the energy lost by the incident electron; for an autoionizing level $\Delta E = E_L$. The corresponding momentum transfer is $K = \sqrt{2\Delta E}$, independent of the initial energy. With these kinematics we measured the (e,e) out-of-plane angular distribution of ejected electrons corresponding to plane III of Fig. 1. This plane contains the momentum transfer vector $\vec{K}$; it is perpendicular to $\vec{k}_{sc}$ and hence also to the scattering plane. (Note that all ejected electron directions $\hat{k}_{ej}$ in plane III are perpendicular to $\hat{k}_{sc}$.) Our experiments were carried out with an incident electron energy $E_0 = 488$ eV and a corresponding scattering angle $\theta_{sc} = 20.5^\circ$ for an energy loss of $\approx 60$ eV and a momentum transfer $K = 2.1$ in the autoionizing region.
We performed three types of calculations for comparison with the experimental data: a simple PWBA calculation and sophisticated first-order and second-order hybrid distorted-wave + convergent $R$-matrix with pseudo-states (close-coupling) calculations (DWB1-RMPS and DWB2-RMPS, respectively). Details of the latter methods are given elsewhere [20, 21, 22, 23]. The essential point is that the (fast) projectile−target interaction is treated perturbatively to first (DWB1) or second (DWB2) order, while the initial bound state and the $e$−He$^+$ half-collision of a slow ejected electron and the residual ion are treated via a convergent close-coupling expansion.

While the PWBA model is not expected to be quantitatively correct, it is useful in that the formalism developed by Balashov et al. [26] makes definite qualitative predictions about the effect of autoionization on the $(e,2e)$ ejected electron angular distributions. For direct ionization, the PWBA and all other theories predict that as $K$ increases the intensity of the recoil peak decreases relative to that of the binary peak, and for the kinematics of the present experiment ($K \approx 2$) it essentially vanishes. However, when autoionization is present the recoil peak remains significant and exhibits a specific shape determined by the angular momentum $L$ of the autoionizing state; each of the three He autoionizing levels ($L = 0, 1, 2$) is expected to leave.
Figure 4. (Color online). Helium out-of-plane ($e_2e$) ejected electron angular distributions for 488 eV electrons scattered through 20.5°. The vertical bars represent the experimental results and include both statistical and systematic errors. (a) Direct ionization with 34.1 eV ejected electrons. (b)–(d) Autoionization via (2s$^2$)$^1S$, (2p$^2$)$^2D$, (2s2p)$^1P$. The solid (red) and dashed (blue) lines are DWB2-RMPS and DWB1-RMPS calculations, respectively, while the chained (green) lines are fitted PWBA calculations described in the text. Theory and experiment are normalized to unity at $\theta_0 = 0$.

a characteristic signature in the shape of a recoil peak with behavior given by the square of the $L^{th}$ Legendre polynomial $P^2_L$ [1]. The scattering amplitude is dependent (when autoionization is present) on $q_L$ – the Fano resonance profile index [24]. In our model, $q_L$ was left as an adjustable parameter to be fitted to the experimental data.

Figure 4 exhibits our experimental results and theoretical predictions; $\theta_0 = 0$ is the binary peak position (i.e., momentum transfer direction) and $\theta_0 = 180^\circ$ is the recoil peak position — all other angles lie outside the scattering plane (see plane III of Fig. 1). All experimental data and the PWBA calculations were normalized to unity at the binary peak. Each set of DWB2-RMPS calculations was fitted to the data using a $\chi^2$ test – the scaling factor was the only parameter for each fit. Each of these scaling factors was also used for the corresponding set of DWB1-RMPS calculations: we are making the assumption that each set of DWB2-RMPS calculations should provide a better description of the experimental data than the corresponding DWB1-RMPS calculations.

Figure 4 (a) is the angular distribution for direct ionization. The PWBA underestimates the width of the binary peak and the DWB1-RMPS overestimates the height of the binary peak,
whereas the DWB2-RMPS calculations are in good agreement with experiment over the entire angular range, within the statistics of the present experiment. The data show conclusively that the recoil peak is extremely small, and we therefore expect autoionization to have a profound effect on this part of the angular distribution.

That this is indeed the case is seen in Figs. 4 (b)–(d), which show the angular distributions of the $^1S$, $^1D$, and $^1P$ autoionizing levels. For the PWBA calculations values of $q_L$ were chosen to give the correct recoil peak intensities. The resultant curves agree quite well with the experimental data, with fitted values $q_0 = -15$, $q_1 = -6.3$, and $q_2 = -4.8$. As predicted, a comparison of the PWBA calculations with the data shows that each autoionizing level has a signature determined by the behavior of the appropriate $P^2_L$. In Fig. 4 (b) the data for $^1S$ are clearly non-zero over the entire angular range, as expected from $P^0_0 = \text{constant}$. Both the $^1D$ and $^1P$ angular distributions in Figs. 4 (c) and (d) show pronounced recoil peaks and minima close to $90^\circ$, and the data in the range $\theta_0 = 60^\circ \rightarrow 135^\circ$ are consistent with the behavior of $P^2_2$ and $P^1_1$, respectively.

Both the DWB1-RMPS and DWB2-RMPS models do a good job describing the $^1S$ data (Fig. 4 (b)). However, the first-order DWB1-RMPS model appears to overestimate the binary peak while slightly underestimating the recoil peak, while the DWB2-RMPS model somewhat underestimates the binary peak. These characteristics become more pronounced for the $^1D$ and $^1P$ angular distributions (Figs. 4 (c) and (d)). It is interesting that while the DWB2-RMPS calculations do better than the DWB1-RMPS calculations at describing the experimental results, the DWB1-RMPS calculations consistently do a better job of describing a large part of the out-of-plane data (i.e., for $\theta_0 = 45^\circ \rightarrow 120^\circ$).

4. Current work

Using an incident electron energy of 488 eV (as for the experiments detailed in the previous sections), we have completed a series of experiments that test details of the theories by measuring ejected electron angular distributions as a function of energy across each resonance. The analysis of this data is ongoing, however, two spectra are shown in figure 5. Both of these spectra are for ejected electron directions along the momentum transfer direction, and scattered and incident electron directions as shown in figure 1.

Currently, we are measuring out-of-plane angular distributions for He direct, and autoionization using 150 eV incident energy electrons. At this incident energy it is expected that exchange effects will become significant. Initial experiments are being done with the same scattered and ejected electron angles as the 488 eV experiments – the kinematics correspond to the plane shown in figure 6. Preliminary experimental results for direct ionization and the $^1P$ resonance are shown in figure 7.

5. Conclusion

In summary, we have measured out-of-plane angular distributions for He direct ionization and three autoionizing levels. For direct ionization, a three-body process, both first-order and second-order distorted-wave calculations give an adequate description, as was true for out-of-plane experiments on Mg [5, 19]. We find that the presence of autoionization has a dramatic effect on the recoil peak, as predicted by Balashov et al [26]. For an incident energy of 488 eV and a momentum transfer of 2.1 au, we find that a second-order model in the projectile–target interaction is necessary to correctly reproduce the magnitude of the recoil peak when autoionization is present; the corresponding first-order model underestimates the magnitude by a factor of three. Similarly the fitted $q$ parameters are larger by factors of between three and eight than first-order calculated values found in the literature [25]. This need for a higher-order description is consistent with recent excitation-ionization experiments (i.e., four-body processes); e.g., [16, 17, 18]. However, neither the DWB2-RMPS or DWB1-RMPS calculations is able to
Figure 5. Coincidence energy spectra showing the $^1S$ (top panel) and the $^1D$ and $^1P$ (bottom panel) resonances. Vertical lines indicate the uncertainty ($\pm \sigma$) in the experimental data. Dashed (blue), solid (red) lines indicate the results of DWB1-RMPS, and DWB2-RMPS (respectively) calculations. See text for further details.

Figure 6. Geometry for the initial 150 eV incident electron energy experiments. See text for details.

Figure 7. Preliminary experimental out-of-plane angular distributions for He direction ionization (left panel) and $^1P$ resonance (right panel) for an incident electron energy of 150 eV. The geometry is as shown in figure 6, with $0^\circ$ and $180^\circ$ corresponding to the binary, and recoil lobes, respectively.

reproduce the data over the full $0 \rightarrow 180^\circ$ out-of-plane range; DWB2-RMPS is good in the recoil peak but bad in the central region, and the opposite is true of DWB1-RMPS. Our overall conclusion is that, for our kinematics, current sophisticated theories can adequately describe out-of-plane experiments on direct ionization (three body dynamics) but are inadequate for equivalent experiments on He autoionization (four body dynamics).

Experimental results that test details of the theories by measuring ejected electron angular distributions as a function of energy across each resonance, are being analyzed. Additionally, we
have begun a series of experiments to measure out-of-plane angular distributions for He direct,
and auto-, ionization at an incident energy of 150 eV.

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