COMPTON IONIZATION OF ATOMS NEAR THRESHOLD AS A METHOD OF SPECTROSCOPY OF OUTER SHELLS

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Kinematically complete experimental study of Compton scattering at helium atoms near the threshold

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General

In general, Compton scattering is a relativistic process. Its theory is well known for a long time and presented in many textbooks. However, if the initial photon energy ω_1 is of the order of a few keV, and the energy of the escaped electron is a few eV (near treshold), the non-relativistic approach is possible. The energy and momentum conservation laws are

$$\omega_1 = \omega_2 + I_p + E_p + E_{ion}, \tag{1.1}$$

$$\vec{k}_1 = \vec{k}_2 + \vec{p} + \vec{K}, \tag{1.2}$$

where I_p is the ionization potential, E_p ($\vec{p}$) is the energy (momentum) of the escaped electron, E_{ion} ($\vec{K}$) is the energy (momentum) of the residual ion, ω_i ($\vec{k}_i$) is the energy (momentum) of the initial (final) photon. The momentum transfer is given by $\vec{Q} = \vec{k}_1 - \vec{k}_2$. We can also rewrite the energy conservation law in a convenient form

$$\omega_2 = \omega_1 \left(1 - \frac{I_p + E_p}{\omega_1}\right) = \omega_1 t, \quad t \lesssim 1.$$

In the non-relativistic energy range we can use the atomic units $e = m_e = \hbar = 1$.In these units, $E_p = p^2/2$, $k_i = \omega_i/c$, $\omega(a.u.) = \omega(keV)/27.2(eV) \sim c\,(= 137)$, so that $k_i \sim 1$ in the chosen photon energy range. In these notations $Q = k_1\sqrt{1 - 2t\cos\theta + t^2}$, θ denoting the angle between the photon momenta $\vec{k}_1$ and $\vec{k}_2$.

Motivation

The main motivation of this investigation was to establish a new method of studying the momentum distribution of the active electron in an atomic target in analogy to the Electron Momentum Spectroscopy (e,2e).

Experiment

Scheme of the experiment

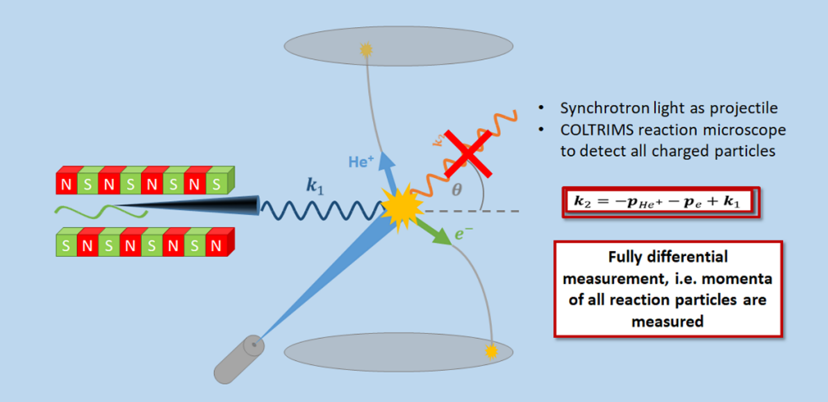
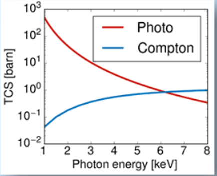


Figure 1:

Problems and challenges

Compton scattering cross section is very low. ($\approx 10^{-24}$cm^2, **one million times smaller** than typical photoionization cross sections!)

The typical solution: **high target density** (solids)



We do a **fully differential measurement**, i.e. all particle momenta have to be detected in coincidence.
Therefor, we need a gas target, i.e. **low target density**

Our solution: **high photon flux**

Figure 2:

Synchrotron light

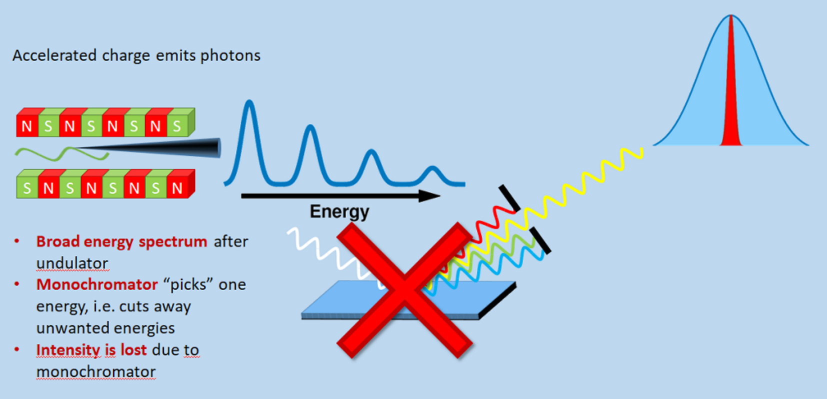


Figure 3:

Theory

Relativistic approach

The problems of relativistic approach within QED:

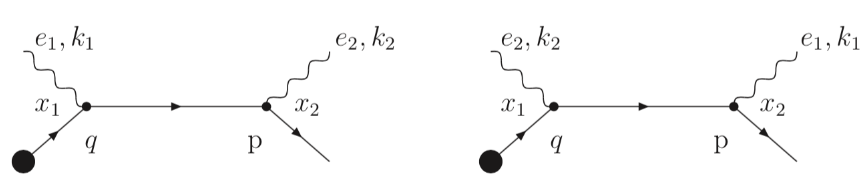


Figure 4:

1. The ion is treated not as a particle, but as the source of an external classical Coulomb field. In COLTRIMS the ion is treated as a particle that moves and acquires a momentum after the interaction.
2. It is extremely difficult to build a correlated wave function of the atomic initial state.
3. It is very difficult to find Green's function of the intermediate virtual electron in the Coulomb field.

Non-relativistic approach

We consider Compton scattering at helium atoms. The non-relativistic TDSE, which describes the atom-light interaction, reads:

$$i\frac{\partial}{\partial t}\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_p,t) = \left[\frac{1}{2}\left(-i\vec{\nabla}_1 - \frac{1}{c}\vec{A}(\vec{r}_1,t)\right)^2 + \frac{1}{2}\left(-i\vec{\nabla}_2 - \frac{1}{c}\vec{A}(\vec{r}_2,t)\right)^2 + \right.$$

$$\left. \frac{1}{8M}\left(-i\vec{\nabla}_p + \frac{1}{c}\vec{A}(\vec{r}_p,t)\right)^2 - \frac{2}{|\vec{r}_p-\vec{r}_1|} - \frac{2}{|\vec{r}_p-\vec{r}_2|} + \frac{1}{|\vec{r}_1-\vec{r}_2|}\right]\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_p,t). \quad (1)$$

In Eq. (4) $M = 1836$ a.u. is the mass of the proton, $\vec{r}_p$ is its coordinate and $\vec{r}_{1,2}$ denote the coordinates of the electrons. The vector potential is defined as follows

$$\frac{1}{c}\vec{A}(\vec{r},t) = \sqrt{\frac{2\pi}{\omega_1}}\,\vec{e}_1\, e^{i(\vec{k}_1\vec{r}-\omega_1 t)} + \sqrt{\frac{2\pi}{\omega_2}}\,\vec{e}_2\, e^{-i(\vec{k}_2\vec{r}-\omega_2 t)}. \quad (2)$$

Here $\vec{e}_1$ and $\vec{e}_2$ are linear polarizations of the initial and final photons. This choice of the vector potential corresponds to a single incident photon and a single outgoing photon. We remind that $(\vec{k}_i \cdot \vec{e}_i) = 0$, so that $\mathrm{div}\vec{A}(\vec{r},t) = 0$ (the Coulomb gauge).

The interaction term of an electron and the photon is written as

$$V_{int} = i\frac{1}{c}\,(\vec{A}(\vec{r},t)\cdot\vec{\nabla}_r) + \frac{1}{2c^2}A^2(\vec{r},t) =$$

$$i\left(\sqrt{\frac{2\pi}{\omega_1}}\;e^{i(\vec{k}_1\vec{r}-\omega_1 t)}(\vec{e}_1\cdot\vec{\nabla}_r) + \sqrt{\frac{2\pi}{\omega_2}}\;e^{-i(\vec{k}_2\vec{r}-\omega_2 t)}(\vec{e}_2\cdot\vec{\nabla}_r)\right) +$$

$$\left(\frac{\pi}{\omega_1}\;e^{2i(\vec{k}_1\vec{r}-\omega_1 t)} + \frac{\pi}{\omega_2}\;e^{-2i(\vec{k}_2\vec{r}-\omega_2 t)} + \frac{2\pi}{\sqrt{\omega_1\omega_2}}\;(\vec{e}_1\cdot\vec{e}_2)\;e^{i[(\vec{k}_1-\vec{k}_2]\vec{r}-(\omega_1-\omega_2)t]}\right). \quad (6)$$

The red term is the well-known Kramers - Heisenberg - Waller matrix element. It is also called A^2 term, which is analogous to the FBA in agreement with the ionization reactions with electrons and bare ions. We focus our attention on considering this term.

In calculating the matrix element we omit the intermediate operations only enumerating them:

1. Because of the huge mass of the alpha-particle we dropped its interaction with the EM field from the total interaction term (6).

2. We integrate the FBA matrix element with respect to time and $\vec{r}_p$, which gives the delta-functions of energy and momentum conservation.

3. We also integrate with the help of these delta-functions.

The full differential cross section (FDCS) in the atomic units can be written as

$$\frac{d^3\sigma}{dE_e d\Omega_e d\Omega_1} = \frac{\alpha^4}{(2\pi)^3}\, p \left(1 - \frac{p^2/2 + I_p}{\omega_1}\right)^2 \frac{1}{2} \sum_{e_1, e_2} |M|^2. \quad (7)$$

The sum in (7) implies the averaging over the initial (linear) photon polarizations and summing over the final (linear) photon polarizations.

$$M(\vec{Q}, \vec{p}) = (\vec{e}_1 \cdot \vec{e}_2) < \Phi_f^-(\vec{p})| \sum_{j=1}^{2} e^{i\vec{Q}\vec{r}_j} |\Phi_0 > . \quad (8)$$

Here $\vec{e}_i$ is the photon polarization vector. We have to remark that the initial $|\Phi_0 >$ and final $< \Phi_f^-(\vec{p})|$ states of the atom must be orthogonal $< \Phi_f^-(\vec{p})|\Phi_0 >= 0$, i.e. $M(0, \vec{p}) = 0$. Thus, if these functions do not belong to the same atomic Hamiltonian, they should be obligatory orthogonalized.

In Eq. (8) $\Phi_0(\vec{r}_1, \vec{r}_2)$ is the trial symmetric helium ground state WF, which may have various degrees of electron-electron correlations, and

$$\Phi_f^{-*}(\vec{p}; \vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}[\varphi^{(*-)}(\vec{p}, \vec{r}_1; Z)\varphi_0^{He+}(r_2) + \varphi^{(*-)}(\vec{p}, \vec{r}_2; Z)\varphi_0^{He+}(r_1)]. \qquad (9)$$

$$\varphi_0^{He+}(r) = \sqrt{\frac{8}{\pi}}\, e^{-2r}, \quad \varphi^{(*-)}(\vec{p}, \vec{r}; Z) = e^{-\pi\zeta/2}\Gamma(1 + i\zeta)e^{-i\vec{p}\cdot\vec{r}}\, {}_1F_1[-i\zeta, 1; i(pr + \vec{p}\cdot\vec{r})].$$

$p\zeta = -Z$, and 1) $Z = 1$, 2) $2 \le Z = Z(r) \le 1$.

The momentum transfer Q should be comparable with the electron momentum p.

Results

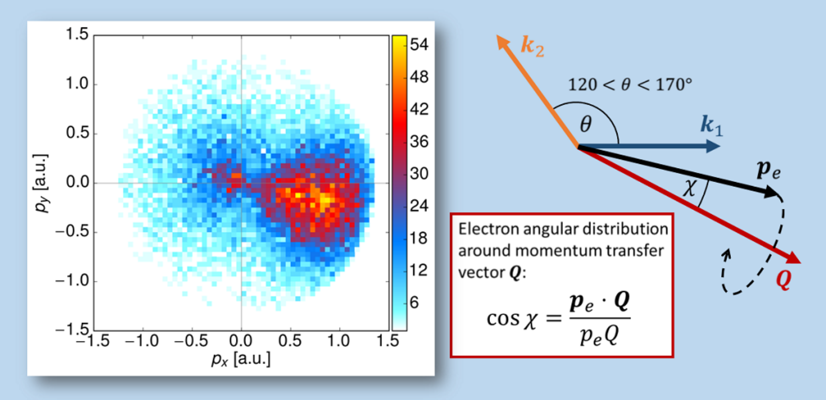


Figure 5:

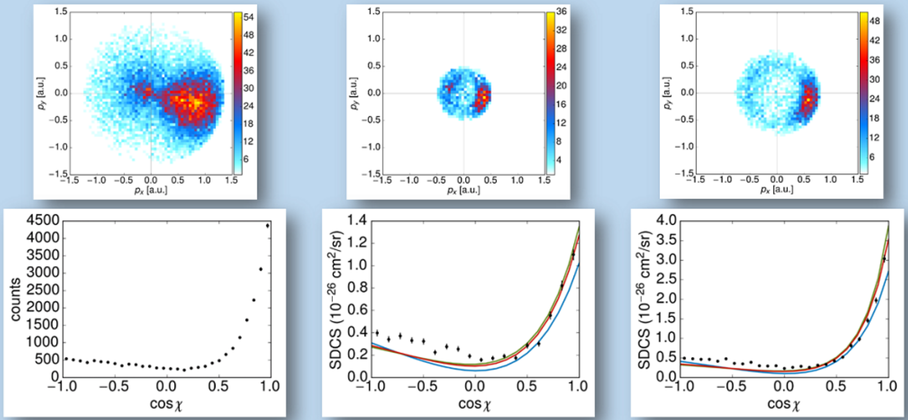


Figure 6:

Fully differential electron angular distributions. The photon scattering angle is $130^\circ < \theta < 170^\circ$. Displayed is $\cos\chi$ between the outgoing electron and the momentum transfer Q for electron energies of a) all energies, b) $1.0 < E_e < 3.5$ eV, and c) $3.5 < E_e < 8.5$ eV.

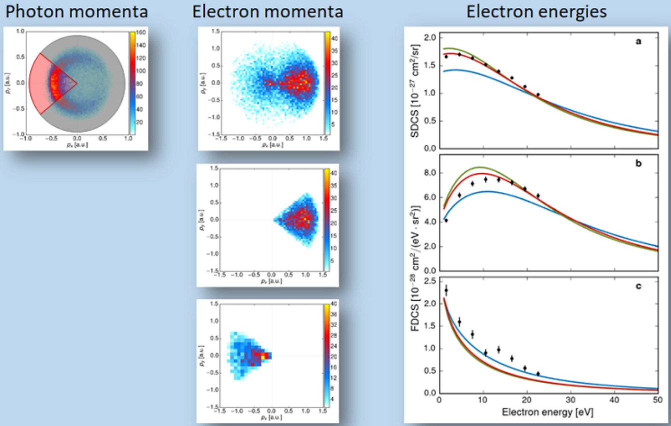

Photon momenta
Electron momenta
Electron energies
SDCS [10^{-27} cm^2/sr]
FDCS [10^{-28} cm^2/(eV · sr^2)]
Electron energy [eV]
a
b
c

Figure 7:

Electron energy distribution. The scattering angle between the incoming and outgoing photon for the outgoing photon is restricted to $140^\circ < \theta < 180^\circ$ in all panels. **a**, The electron energy spectrum is shown independent of the electron emission direction. **b**, The electron emission angle is restricted to forward scattering ($0 < \theta_e < 40^\circ$). **c**, The electron emission angle is restricted to backward scattering ($140^\circ < \theta_e < 180^\circ$). The black dots are the experimental data. The error bars represent the standard statistical error. The solid lines are different theoretical results. The experimental data in a and b are normalized such that the maximum intensity is 1; the theory is normalized such that the integrals of the experimental data and the theoretical curves are equal. The normalization factors in c are identical to those in b, because here we depict the forward/backward direction of the same distribution.

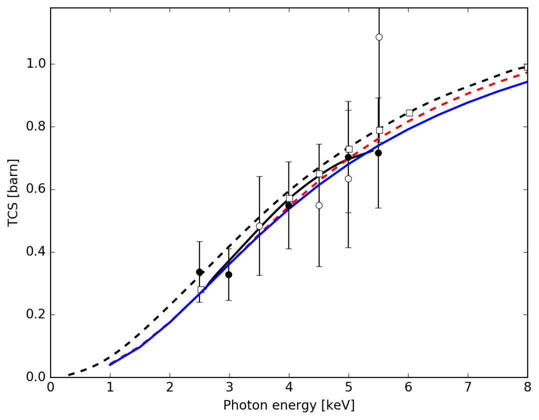


Figure 8: TCS eq. (11) versus the photon energy. Red dashed line: Hy, blue solid line: CF (practically coincides with SPM). Experimental points and other calcs are taken from J.Samson et al, PRL **72** (1994), 3329

Concluding remarks

- Experimental and theoretical perspectives of Compton double ionization;
- Compton scattering on three-body nuclear target;
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Thank you for your attention !