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Names and affiliations of applicants (* indicates experimentalists):
S. Manninen*, Sz. Galambosi*, K. Hämäläinen*, S. Huotari*

Division of X-ray Physics, Department of Physical Sciences,
FIN-00014 University of Helsinki, Finland

Report:

Compton profiles of noble gases from He to Xe ($Z = 2$–54) were measured using a intermediate-pressure gas cell specifically designed for Compton scattering studies. The applied pressure was 50 bar for He, Ne and Ar, 40 bar for Kr and 10 bar for Xe. The pressure, and thus the density of the sample, was optimized to maximize the Compton count rate. These modest pressures naturally do not affect the electronic structure of the sample. The incident photon energy was 56 keV and the momentum resolution about 0.3 atomic units (a.u.). The achieved resolution was lower than in solid-state experiments due to the source size effect, which in the pressurized gas-cell system is more difficult to minimize than in solid-state samples. A second factor that makes the experiments difficult and requires a third-generation synchrotron radiation source, is the low Compton-scattering cross-section, and the high statistical accuracy needed for the analysis of Compton profiles. Accumulated counts at the Compton profile peak varied between 5000–40000 due to very different cross-sections for different gases, so the achieved statistical accuracy varied from 0.5% (Ar) to 1.7% (Xe). Estimations of the contribution of multiple scattering were computed by a Matlab-based software developed by the authors. This contribution was found to be minimal due to low densities of the samples, well collimated incident beam and the focusing spectrometer.

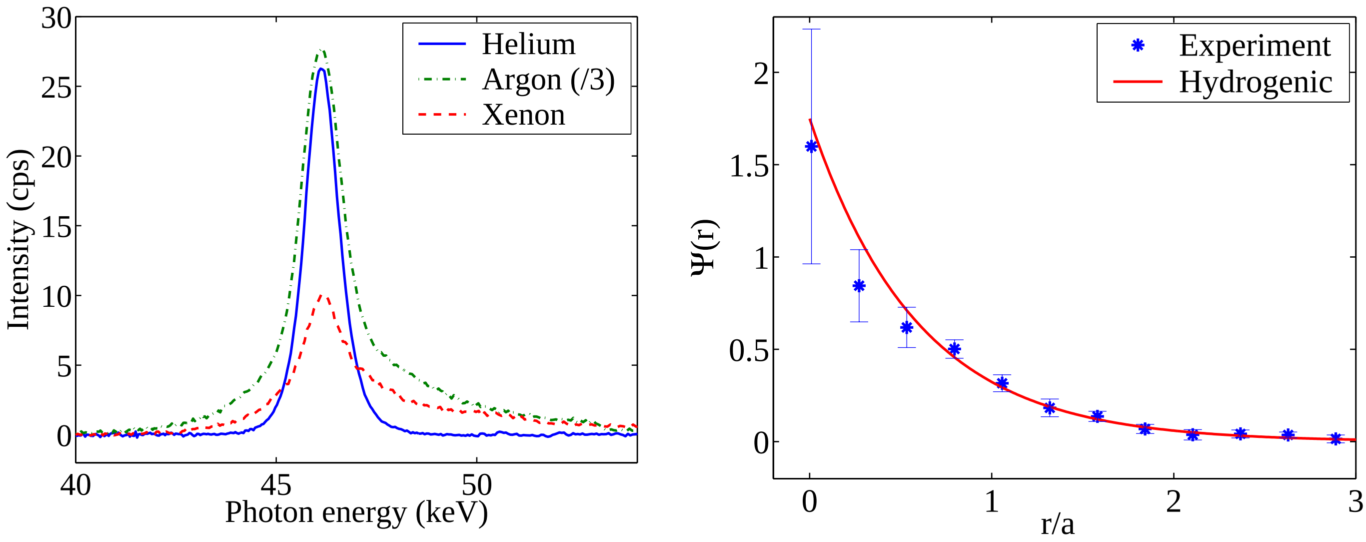

Figure 1. Left: Spectrum of x rays scattered from helium, argon (intensity divided by a factor of 3), and xenon. Right: The extracted real-space single-particle 1*s* wave function of He.

X-ray spectra from some reprensentative cases, namely helium, argon and xenon, are presented in Figure 1 (left panel). In the case of helium, the simplicity of the system allows a very precise theoretical Compton profiles to be calculated. Furthermore, correlation effects were found out to be negligible in the Compton profile of noble gases. In the abscence of correlation, the many-particle atomic wave function can be approximated as a Slater determinant of one-particle wave functions. Utilizing this, we have been able to compute the approximate *real-space* single-particle wave function of He directly from its Compton profile. The results are plotted in Figure 1 (right panel).

As expected, relativistic effects are pronounced in the Kr and Xe Compton profiles. The magnitude of the relativistic effects at the moment relies on computations performed with two different methods, namely *ab initio* (relativistic) and LCAO (non-relativistic) schemes. The comparison shows notable differences between relativistic and non-relativistic Compton profiles of Kr and Xe, but the differences can arise also from using different methods. New computations to study the relativistic effects consistently using the same method and software are currently being planned.