Elastic x–ray scattering by neutral atoms: Outer–shell effects *

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With the recent progress in the setup of high brilliance third–generation synchrotron facilities, new opportunities arise to study the elastic scattering of x–rays by heavy atoms. For photon energies below 1 MeV, the main contribution to this elastic processes arises from the interaction of x–rays with bound atomic electrons. This so–called *Rayleigh* scattering attracts considerable attention as a valuable tool for studying the relativistic, many–body and even quantum electrodynamics (QED) effects in many–electron systems. During the last decades, a large number of experiments have been performed to explore the Rayleigh process for a wide range of photon energies and for various targets. In 2012, for example, the elastic scattering of (linearly polarized) hard x–rays by gold atoms has been observed at the PETRA III synchrotron facility in DESY [1]. To better understand the outcome of this experiment, a theoretical investigation of the elastic $\gamma + A \rightarrow \gamma + A$ process is required which would account for both the many–body phenomena and the relativistic non–dipole contributions to the electron–photon interaction.

The theoretical analysis of the elastic Rayleigh scattering is usually performed within the framework of the second–order perturbation theory. In this approach, all the properties of the scattered light can be expressed in terms of the transition amplitudes [2, 3]:

$$\mathcal{M}(\omega) = \sum_{\nu} \frac{\left\langle \psi_i \left| \hat{\mathcal{R}} \right| \psi_\nu \right\rangle \left\langle \psi_\nu \left| \hat{\mathcal{R}} \right| \psi_i \right\rangle}{\epsilon_i - \epsilon_\nu \pm \hbar\omega} , \qquad (1)$$

where ψ_i and ϵ_i are the (many–body) wave-function and the energy of the atomic state *before* (as well as *after*) the scattering, $\hbar\omega$ is the photon energy, and $\hat{\mathcal{R}}$ is the electron–photon interaction operator. In Eq. (1), moreover, the summation $\sum_\nu$ runs over the *complete* spectrum of an atom, including not only bound– but also positive and negative energy continuum–states. In order to perform this non–trivial summation over *many–electron* states we employed the independent particle approximation (IPA) in which the photon is scattered by a single (active) electron at a time, while the remaining electrons are kept "frozen" [2, 4].

By making use of Eq. (1) and the independent particle approximation, we have explored the elastic scattering of (completely linearly) polarized x–rays by heavy atoms [4]. In this study, special attention was paid to the question of how various atomic shells contribute to the Rayleigh process. In Fig. 1 we display, for example, the angle–differential Rayleigh cross section for the led target and the incident radiation with energy $\hbar\omega = 145$ keV. In our calculations, we have restricted the summation over the occupied electron shells to the K (red dotted line), KL (maroon dash–dotted line), KLM (green dash–dot–dot line), KLMN (blue dashed line) and the KLMNO shells (black solid line). As seen from the figure, the x–ray scattering by weakly bound outer–shell electrons may dramatically affect the differential cross section. The most pronounced effect can be observed at forward scattering angles, where the cross section is enhanced by more than two orders of magnitude if the interaction of incident radiation with (sub–) valence electrons is taken into account. We argue, therefore, that the angular–resolved measurements of the elastic Rayleigh process, as currently performed at the PETRA III facility, may provide valuable information about electronic shell structure of heavy atoms.

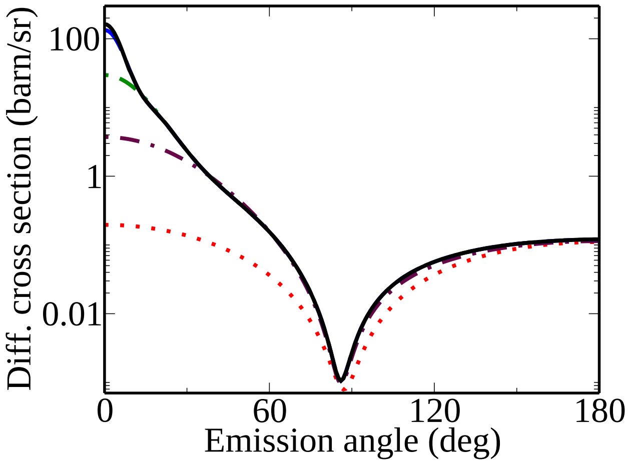

Figure 1: The angle–differential cross section for the elastic scattering of linearly polarized photons with energy $\hbar\omega$ = 145 keV by neutral lead atom. Calculations have been performed within the framework of the independent particle approximation and by taking various atomic shells into account. See text for further details. Data from Ref. [4].

References

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