Relativistic Effects in Photoionization of Outer *ns* Subshells of Heavy Atoms

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Synopsis Dynamic changes due to relativity are very prevalent effects in the photoionization of heavy atoms. Presented is an exploration of the evolution of these dynamic changes as the nuclear charge, Z, increases and how they affect the cross sections.

At high enough Z, relativistic effects become important contributors to the quantitative and qualitative nature of atomic properties. It is important to identify and study these relativistic effects as they evolve with increasing Z in order to fully understand atomic properties. The most prevalent relativistic effect is the creation of spin-orbit doublet channels and dynamic changes, i.e., changes in the wave functions, which also shifts the thresholds. The *ns* subshells are chosen because they do not have a spin-orbit doublet, which simplifies the study of the dynamic effects.

A theoretical study of the 6s subshell of mercury (Z = 80), radon (Z = 86), radium (Z = 88) and nobelium (Z = 102) and the 7s subshell of radium and nobelium have been performed using the relativistic random phase approximation (RRPA) methodology [1]. In order to determine which features in the photoionization cross section are due to relativistic effects, calculations are performed using the (nonrelativistic) random phase approximation with exchange (RPAE) methodology [2]. The RPA methodologies were chosen because of their ability to exclude channels from the calculations. This is important because interchannel coupling can obscure and diminish the dynamic effects. Calculations are performed with and without interchannel coupling for comparisons.

Without the inclusion of interchannel coupling there is a very clear difference between the RRPA and RPAE results, the absence of a Cooper minimum from the RRPA curves, which is clearly present in the RPAE results. As Z increases the Cooper minimum, in the RPAE, falls into the discrete spectrum, as can be seen in top plot of Figure 1(A). Studying the descent of the minimum into the discrete spectrum reveals that the Cooper minimum is clearly missing in the RRPA results and not just hidden in the autoionization region. Interchannel coupling pulls some of the Cooper minimum back out of the discrete, in the RPAE curve (see B plot of Figure 1), and induces one due to the coupling with the 5d subshell in the RRPA curve. The influence of the 5d subshell completely reshapes the two methodologies results into very similar cross sections. The major differences in the (B) bottom plot of Figure 1 are due to the differences between their 5d cross sections.

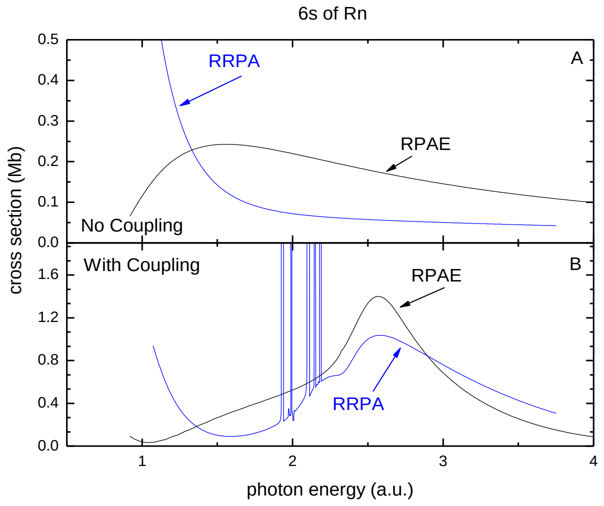

Figure 1 Photoionization cross section of the 6s subshell of radon with (A) and without (B) interchannel coupling included.

References

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