Interchannel Coupling in the Photoionization of Atoms and Ions in the X- Ray Range

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Photoionization cross sections of atoms and ions are of great importance in astrophysical modeling. Since experimental cross sections for most species of astrophysical interest are not yet available, a great deal of effort has gone into the calculation of these cross sections and the associated ionization rates, e.g., the Opacity Project [1], using highly sophisticated theoretical methodologies which include extensive accounting for electron-electron correlation effects. These efforts are confined almost exclusively to outer and near-outer shells of the relevant atoms and ions; the inner shell photoionization data complilations are primarily results of using very much simpler independent particle model (IPM) calculations [2]. This is the data base used in connection with the virtually laboratory-quality data in the x-ray region produced by the recently-launched CHANDRA mission, and other x-ray astronomy missions. Of significance in this regard, however, it has been recently shown that electron- electron correlation is not unimportant for photoionization at x-ray energies or for inner shells [3,4]. In fact it has been found that electron-electron correlation, in the form of interchannel coupling [5], is important for most subshells, of most atoms, at most energies [6]. Basically what is found is that when there is a photoionization channel with a large cross section degenerate with a channel with a small cross section, interchannel coupling can modify the cross section of the channel with the smaller cross section significantly. Electron-electron correlation in atoms and ions is a result of the Coulomb interaction between the pairs of atomic/ionic electrons. With increasing stage of ionization, however, this interelectron Coulomb interaction becomes increasingly less important as compared to the nuclear Coulomb interaction.

To understand how this interchannel coupling, so important in neutral atoms, applies to positive ions, a research program has been initiated to deal with this question, i.e., a program to quantify the effects of interchannel coupling in ionic photoionization, thereby assessing existing photoionization data bases in the x-ray region. To accomplish this task, we have employed the Relativistic Random-Phase-Approximation (RRPA) methodology [7,8] which includes significant aspects of electron-electron correlation, including interchannel coupling. The RRPA methodology has been found to produce excellent agreement with experiment for neutral Ne at photon energies in the 1 keV range [3]. Specifically, it was found the the ratio of the $2s$ to $2p$ photoionization cross sections is altered by interchannel coupling as much as about 40% for 1.5 keV photons as compared to a similar calculation that ignored interchannel coupling. In the keV energy region the $2s$ cross section is significantly larger than the $2p$ since the $2s$

cross section falls off with energy much more slowly than the $2p$ [9]. The "real" wave functions for the $2p$ photoionization channels contains a small admixture of the wave functions of the $2s$ photoionization channels. And, since the $2s$ cross section dominates here, this small admixture leads to a significant alteration of the $2p$ cross section, producing the results discovered earlier [3]. It is also worthwhile to point out that the Ne I calculation showed that the cross section ratio calculated with fully coupled channels, as compared to the result which omits channel coupling, diverge from each other with increasing energy. In other words, the effect seen for Ne I in the 1 keV photon energy region becomes more and more pronounced with increasing energy.

Calculations have been performed on the neon isoelectronic sequence as a test case to illustrate the behavior of interchannel coupling with increasing stage of ionization. Specifically, we have investigated every member of the sequence form neutral Ne I to neon-like Fe XVII. Photon energies from the first $2p$ threshold to at least 25 times the threshold energy were considered; this meant going up to over 30 keV in Fe XVII. In each case two calculations were performed, as was done previously for neutral Ne [3]. In one calculation, a full RRPA was done, with all of the channels coupled. In the second, the coupling among channels arising from different subshells, $2p$, $2s$ and $1s$ for the case of neon-like systems, was omitted to spotlight the effect(s) of this coupling.

The results show that at the higher energies, the interaction of the larger $2s$ cross section with the smaller $2p$ cross section modifies the former by a factor of about 1.4 in neutral neon. Along the isoelectronic sequence, the calculation shows that this modification decreases monotonically to about 1.1 in neon-like iron at the highest energies considered. However, in each case, the fully coupled ratios are diverging from the ratios calculated without channel coupling with increasing energy, just as was the situation for Ne I. It is interesting to note that the influence of correlation upon many other ionic properties does not decrease smoothly as a function of the stage of ionization [10,11] as it appears to here. In any case, based upon these results, our preliminary conclusion is that interchannel coupling must be taken into account for the photoionization of neutral and low-charge ions, and becomes less and less important as the ionic charge increases, but more and more important with increasing photon energy. Several other cases need to be investigated before we can confirm this tentative conclusion. Such studies are in progress.

Finally, it is worthwhile to point out how this results affect the modelling of astrophysical plasmas. It is clear from the above discussion that the coupling of channels can strongly affect the photoionization cross sections of weak channels that are degenerate with cross sections from much stronger channels. Since it is only the small cross sections that are significantly affected, the total photoionization cross section is not changed very much by this interchannel coupling effect. But, for inner shell photoionization, the response to the creation of an inner shell vacancy of an ion in an astrophysical plasma, e.g, x-ray or Auger electron emission, depends critically upon the specific subshell in which the vacancy is created. Thus, small cross sections become important because they populate different states, and produce differing x-ray energies, from their larger counterparts. Furthermore, this alteration of cross sections has an equal effect of the astrophysically-important inverse process, radiative recombination; both the probability of producing certain recombined states, as well as the details of the recombinationation radiation in the x-ray region, can be significantly affected. Thus, to understand the basic physics of the astrophysical plasma, as regards the x-ray region, a quantitative understanding of all inner shell photoionization cross sections of any reasonable size is required, not just the largest ones, particularly as the higher x-ray energies become important in a particular astrophysical situation.

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