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Multiple minima in ground-state photoionization: Interchannel coupling at high Z

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The photoionization of the 7*s* subshell of Ra has been investigated using a 20-channel relativistic random-phase-approximation calculation. The results show that in addition to the "natural" Cooper minimum, there are two others induced by interchannel coupling with the 6*p* and 5*d* photoionization channels. This result has important consequences for photoelectron angular distributions as well as excited-state photoionization for high-Z atoms.

Photoionization of outer atomic subshells is affected significantly by the existence of Cooper minima.[1] Cross sections, photoelectron angular distributions, and branching ratios all show large effects when minima are present[2,3] for high-Z atoms. The situation is even more dramatic as the nonrelativistic Cooper minima are split into two (for initial *s* states) or three minima under the influence of relativistic interactions.[2,3]

These minima show up generally in the one-electron central-field[4] or Hartree-Fock[5] calculation, but their location and shape are often strongly affected by interchannel coupling. In some instances, such as Xe 5*s*, the minimum is induced entirely by interchannel coupling.[6] In at least one case, that of Ca 4*s*, there is one minimum in the one-electron calculation (a "natural" minimum) and a second induced by interchannel coupling with the 3*p* photoionization channels.[7] Thus it is not only in excited-state photoionization that multiple minima can occur.

For high-Z atoms there are more occupied subshells, enhancing to possibilities for interchannel interactions. Furthermore, the strength of the relativistic interactions splits these minima, making their effects more noticeable in the photoelectron angular distribution asymmetry parameter β. For these reasons, we have investigated the photoionization of radium, $Z=88$. We have focused particularly on the 7*s* subshell, whose β would be 2 in the absence of relativistic effects; even with relativity β would not deviate much from 2 if no Cooper minima were present.[8]

We have preformed a relativistic random-phase-approximation (RRPA) calculation[9] of the Ra 7*s* photoionization, including coupling between all of the relativistic dipole-allowed channels arising from 7*s*, 6*p*, 6*s*, 5*d*, and 5*p*; a total of 20 channels. The RRPA methodology has been shown to give excellent agreement with experiment for the outermost subshell in a number of cases at lower Z. This further dictated our choice of the 7*s* to study, the 7*s* being the outermost subshell.[6]

The calculated photoionization cross section for Ra 7*s* is shown in Fig. 1 in both length and velocity formulations. Clearly this is not a simple cross section. Minima are seen at photon energies of about 0.4, 1.8, and 5.2 a.u. Both length and velocity cross sections are shown with the agreement between them becoming steadily worse as energy increases and the effects of the omitted channels become more important.

To investigate the origin of the structure in this cross section, some tests were run. Coupling in only the 7*s* channels leads to a cross section which has the high-energy minimum, but is monotone decreasing from threshold at lower energies. This clearly points to interchannel coupling as the origin of the lower-energy structure. In fact, further tests have shown that the structure below 1 a.u. is due to interchannel coupling with the 6*p* channels, while the minimum just below 2 a.u., and the maximum above it are due to coupling with the 5*d* channels. This is to be expected as the 6*p* channels open around 1 a.u. and the 5*d* around 3 a.u. Then, since these channels have their maximum cross section near threshold one would expect the

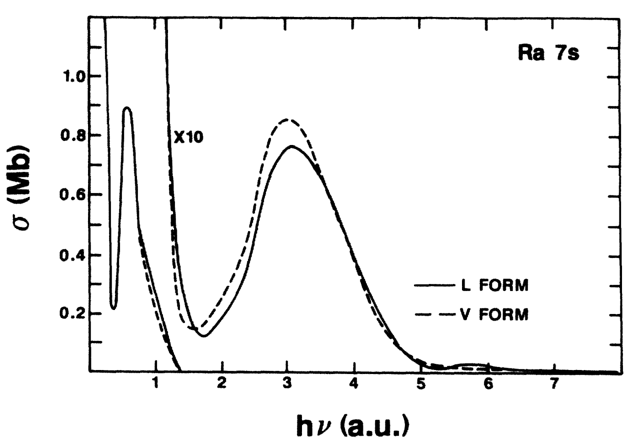

FIG. 1. Photoionization cross section for Ra 7*s* calculated in a 20-channel RRPA. Both length (L) and velocity (V) forms are shown.

largest interchannel effects there.

But are the minima seen really Cooper minima? That is, do they indicate a change of sign of the matrix element? To check this point, one can look at the photoelectron angular distribution. A transition from an s subshell can go to a $p_{1/2}$ or $p_{3/2}$, and the asymmetry parameter β for a closed shell system is given by[8]

$$\beta = \frac{2R_{3/2}^2 + 4R_{1/2}R_{3/2}\cos(\delta_{1/2}-\delta_{3/2})}{R_{1/2}^2 + 2R_{3/2}^2} , \qquad (1)$$

where R_j are the dipole matrix elements to the εp_j continua, and δ_j are the phase shifts. Now the phase shifts are generally quite close so that the cosine is quite close to unity. Thus, if $R_{1/2}$ and $R_{3/2}$ are close in value, $\beta \approx 2$, independent of energy or the variation of the R_j with energy. If, however, there is a Cooper minimum, the value of β will differ markedly from 2; from Eq. (1) it is seen that where $R_{1/2}=0$, $\beta=1$, and where $R_{3/2}=0$, $\beta=0$. Between these two values, inspection of Eq. (1) shows that β goes negative; in fact, to -1. In a calculation including interchannel coupling, the situation is modified slightly by the fact that the matrix elements are complex and the real and imaginary parts vanish at different (but very close) energies. This means that a true Cooper minimum never exists, but the matrix element comes close enough to zero for all practical purposes.

In any case, our calculated β is given in Fig. 2, where it is seen that β comes close to -1 near each of the minima in the cross section. This confirms that they really are Cooper minima. In addition, away from the minima, β tends toward 2, just as predicted above. Further, from the width of the dips one can determine the splitting between the $p_{1/2}$ and $p_{3/2}$ minima in each case. For the lowest energy dip, the splitting is ~0.2 a.u., the middle one ~0.5 a.u. and the highest energy dip, where the length-velocity disparity becomes large because of truncation, > 3 a.u.

The consequences of this result are not limited to the photoionization of Ra 7s. The phenomenology found will be qualitatively true for all outer s subshells of high-Z atoms. In addition, and perhaps more important, this will extend to excited states as well. Previously, it was found that the maximum number of minima in the dipole matrix element for a given ionizing transition is three,[10] but interchannel coupling of the type discussed above could increase that number. Furthermore, since sum rules must still be obeyed, diminution of the oscillator strength in a particular spectral region must be matched by an increase elsewhere. Thus the existence of these "induced" minima can cause a change in the photoionization cross section over a broad energy region.

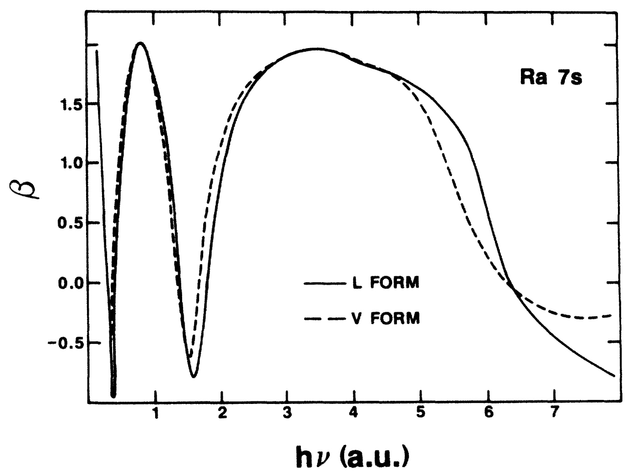

FIG. 2. Photoelectron angular distribution parameter for Ra 7s calculated in a 20-channel RRPA. Both length (L) and velocity (V) forms are shown.

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