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Brief Reports

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Near-threshold structure in the photoionization of krypton 3*p*

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Calculations of the photoionization cross section of Kr 3*p* have been performed at four different levels of approximation, from the central-field Hartree-Slater to the 20-channel relativistic-random-phase approximation. The results show unequivocally that the structure that appears at the central-field level is not an artifact of the calculation but persists through the most sophisticated level of approximation.

Nonresonant oscillations in photoionization cross sections have been the subject of considerable scrutiny of late.[1,2] Aside from structure in the cross section arising from a zero in the dipole matrix element, known as a Cooper minimum,[3] other structures were predicted by calculations some time ago[4] and later studied in more detail.[5] Recently, however, it has been shown that some of this other structure is simply an artifact of the model potential employed.[1,2] In this paper it is shown that not all such structure is model dependent.

In particular, these oscillations and structures were first found in simple Hartree-Slater (HS) calculations in the region above inner-shell ionization thresholds;[4] these oscillations appeared in HS calculations even of *K*-shell photoionization and generalized oscillator strengths.[5,6] These HS calculations include the Latter tail[7] in the potential which generates a discontinuity in the derivative of the potential. Recent work has shown that this discontinuity leads to oscillations in the dipole matrix element and, hence, the photoionization cross section.[2] There are, nevertheless, nonresonant structures which are not Cooper minima that are not related to the Latter tail.

To demonstrate the point unequivocally we present calculations of the photoionization of the 3*p* subshell of Kr in the region of threshold at several different levels of approximation; HS, Hartree-Fock (HF), intrachannel (5-channel) relativistic-random-phase approximation (RRPA), and 20-channel RRPA. Certainly, if the effect persists through all of these levels of approximation it cannot be model dependent.

The results are shown in Fig. 1. The HS calculation[4] shows a rise from threshold, followed by a dip, then a

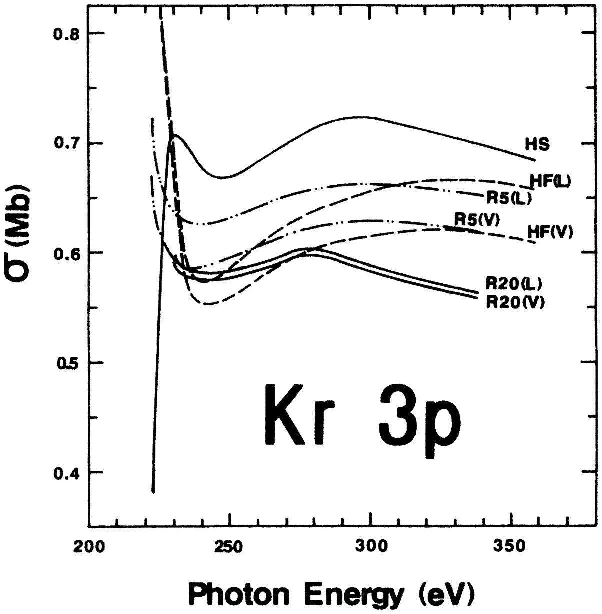

FIG. 1. Photoionization cross section of Kr 3*p* calculated in Hartree-Slater (HS), Hartree-Fock (HF), 5-channel RRPA (R5), and 20-channel RRPA (R20) approximations; the *L* or *V* indicate length and velocity formulations, respectively. To facilitate comparison, all theoretical curves have been translated to the mean experimental threshold of 230.38 eV (Ref. 11). This entailed shifting HS and HF curves 14.72 eV to the right, while the RRPA curves were shifted 12.08 eV to the left. The shifts amount to comparing the results as a function of photoelectron energy. HF(*L*) and HF(*V*) are 0.85 Mb and 0.83 Mb at threshold, respectively.

rise, and the eventual fall off of the cross section some 60 eV above threshold. The HF results,[8] given in both length and velocity form, show a marked drop from threshold, followed by a rise to maxima about 100 eV above threshold, before the eventual fall off. The 5-channel RRPA cross sections, which include only interchannel interactions within the 3*p* subshell and also shown in length and velocity, are rather similar to the HF results with the drop somewhat less pronounced and the second maximum closer to threshold. Finally, the 20-channel RRPA results, which include coupling between all of the channels arising from 3*s*, 3*p*, 3*d*, 4*s*, and 4*p* photoionization, are similar to the 5-channel results; the second maximum in the cross section is at lower energy and is not as pronounced, however. Note that length and velocity, which show noticeable disagreement at the HF and 5-channel RRPA level, are virtually identical for the 20-channel RRPA, indicating the quality of this calculation. Note further that the 20-channel RRPA results are not shown down to threshold to avoid confusion in Fig. 1; they do, however, merge with the 5-channel RRPA velocity results in the threshold region.

It is important to emphasize that the bulk of the oscillations in the curves shown in Fig. 1 occur in energy regions where the phase shifts of the final continuum states are smooth, i.e., nonresonant. Actually, the initial rise of the HS cross section is the tail end of a shape resonance; the *d*-wave phase shift changes by about $\pi/4$ in the first 10 eV above threshold.[4] Above this energy, where most of the oscillations occur, the phase shift is flat as a function of energy.[4] Thus the structure seen in the HS result is not a resonance phenomenon. The HF *d*-wave phase shift changes only by about $\pi/10$ in this energy region[8] and the RRPA phases change by even less than that; there too, then, the structures are not resonances.

While it is true that the Latter tail can generate oscillations,[1,2] it does not follow that all oscillations are caused by the Latter tail. Neither the HF nor RRPA calculations include the Latter tail. Nevertheless, the structure in the HS is reproduced qualitatively in both the HF approximation and RRPA, showing conclusively that the structure in the 3*p* photoionization cross section *cannot* be an artifact of the Latter tail.

We explain this behavior of the cross section in terms of the behavior of the amplitude of the continuum wave function, εd in this case, which is given for small r as

$$P_{\varepsilon l}=C_{\varepsilon l}r^{l+1} . \tag{1}$$

The photoionization cross section can be written as

$$\sigma=|C_{\varepsilon l}|^2\bar{\sigma} , \tag{2}$$

where $\bar{\sigma}$ is a *reduced* cross section. The crucial point is that $\bar{\sigma}$ is monotone decreasing for all of the curves shown in Fig. 1; the structure is caused by variations in the amplitude factor $C_{\varepsilon d}$ with energy. Physically, the variation of this amplitude factor can be thought of as the result of the diffraction of the emerging photoelectron through the atomic field.[9] This amplitude factor has been studied in some detail recently.[10]

In conclusion, then, we have shown by explicit calculation on Kr 3*p* that oscillations in photoionization cross sections not associated with resonance behavior or Cooper minima have a physical basis and are not necessarily artifacts of the calculation. Unfortunately, while experimental data on Kr 3*p* exist,[11] only three points are in the energy region covered by Fig. 1; these data are insufficient to confirm or deny the predicted structure. Finally, we note that a recent study[12] has detailed the structures that result from a discontinuity in the derivative of the potential. In addition it was found that while removal of the discontinuity eliminated a number of the structures, others remained, in agreement with the present results.

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