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Photoionization of the Cs 6*d* excited state

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Hartree-Fock calculations of the photoionization of the Cs 6*d* excited-state cross section are presented which quantitatively revise previous central-field estimates and bring the results into agreement with experiment.

In recent years various calculations have predicted the existence of multiple minima in the photoionization of excited states of atoms.[1-4] Particularly striking have been the minima in excited *d* states due to zeros in the $nd \rightarrow f$ dipole matrix elements. These minima are extremely sensitive to the details of the initial- and final-state wave functions employed in the calculation and, as such, provide an excellent test of the wave functions when compared with experiment.

A recent experiment[5] has searched for such a minimum in the photoionization of the excited 6*d* state of Cs and found no indication of a minimum at the energy predicted by a Hartree-Slater (HS) central-field calculation.[6] In this paper we examine this discrepancy and present more accurate Hartree-Fock (HF) calculations of the Cs 6*d* photoionization cross section.

The calculation was performed using a discrete HF Cs 6*d* numerical wave function generated by standard code.[7] We have found that numerical wave functions are far superior to parametric wave functions owing to the sensitivity of the minimum to the details of the wave function. This matter is discussed in detail elsewhere.[8] The final ionic state was obtained in the same way and the continuum wave functions were obtained in the field of the Cs^+ HF orbitals using our own code;[9] the details of this continuum HF calculation have been reported earlier.[9] The HF calculations were carried out in both length and velocity formulations.

The resulting cross sections are shown in Fig. 1, along with the HS result.[6] Several things are immediately apparent from these results. First is that the HS calculation finds the minimum just above 0.1 Ry above threshold, while the HF results (both length *and* velocity) find the minimum at about 0.95 Ry. Second is the fact that despite

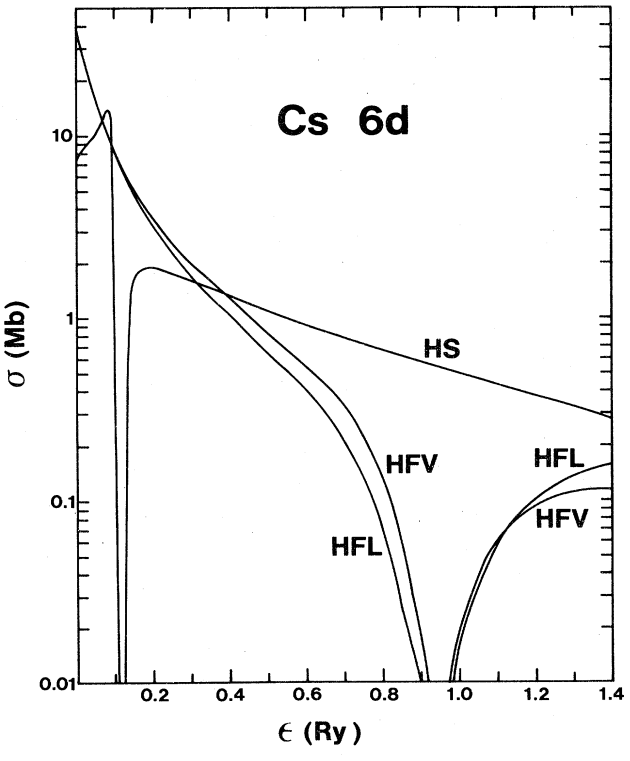

FIG. 1. Cross section for Cs 6*d* photoionization in Hartree-Fock length (HFL), Hartree-Fock velocity (HFV), and Hartree-Slater (HS) approximations. The HS result is from Ref. 6.

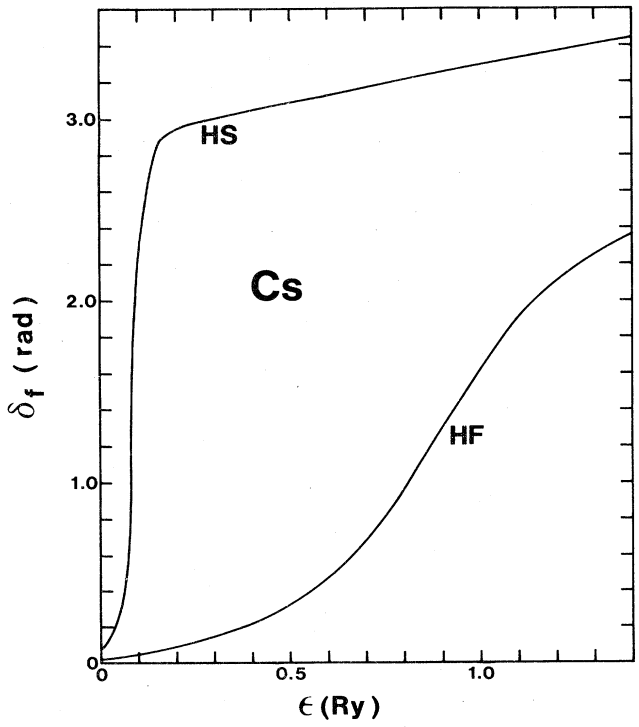

FIG. 2. *f*-wave phase shift in Hartree-Fock (HF) and Hartree-Slater (HS) approximations. The HS result is from Ref. 10.

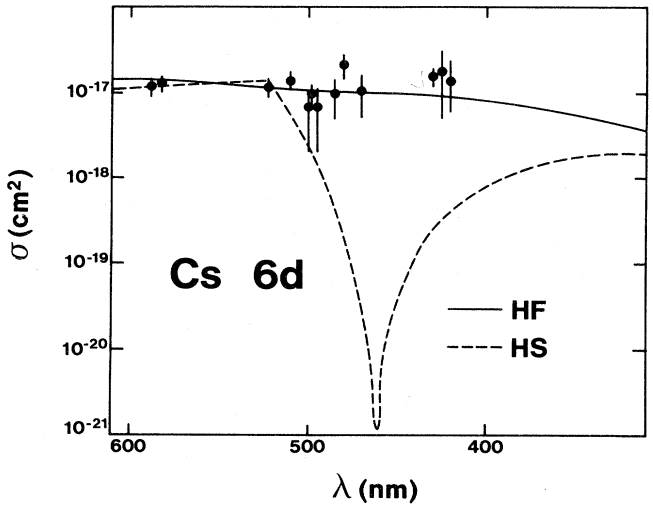

FIG. 3. Photoionization cross section for Cs 6d in Hartree-Fock (HF) and Hartree-Slater (HS) approximations. The HS result is from Ref. 6 and the experimental points are from Ref. 5. Only a single HF curve is shown because length and velocity almost coincide in this region.

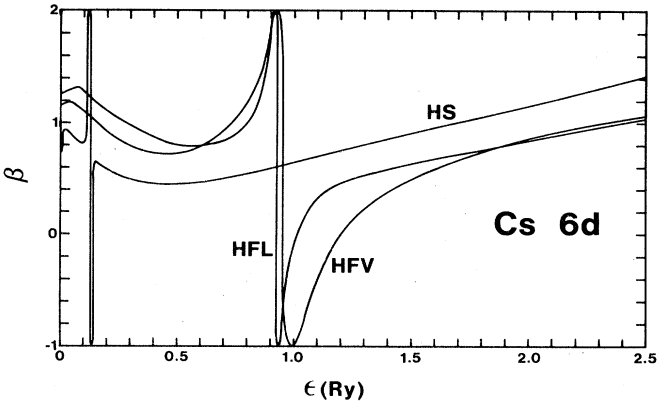

FIG. 4. Photoelectron angular-distribution asymmetry parameter β for Cs 6d in Hartree-Fock length (HFL), Hartree-Fock velocity (HFV), and Hartree-Slater (HS) approximations. The HS result is from Ref. 6.

the quantitative differences between HF and HS cross sections, they still have the same general qualitative structure, large at threshold, dropping off to a minimum and subsequent rise. Third is that the rather good agreement between the HF length and velocity cross sections is indicative of the accuracy of the HF results.

The principal reason for the quantitative difference between the HF cross section on the one hand and the HS result on the other is connected to the shape resonance in the $6d \rightarrow \epsilon f$ channel. The phase shifts showing the shape resonances are given in Fig. 2 where it is seen that δ_f(HS) rises much more rapidly[10] and at significantly lower energy than does δ_f(HF). This means that the ϵf wave function moves in toward the nucleus much more rapidly with energy in the HS case than for the HF formulation. Thus the proper overlap with the discrete 6d wave function is reached at a much lower energy in the HS case; in fact, it is seen that the most rapid rise of the phase shifts in Fig. 2 correlates well with the position of the minima in Fig. 1. This also explains the narrowness of the HS minimum compared with the HF. Near the minimum, δ_f(HS) is rising extremely rapidly. Thus the HS ϵf wave function is moving in rapidly with energy and the matrix element goes through its zero and "recovers" in a small energy range. The same argument shows that in the HF case where δ_f(HF) rises much more gradually the drop and subsequent recovery occurs over a much larger energy range.

The measurement that has been made was only over a small energy region and was a relative measurement.[5] In Fig. 3 the cross section in HF and HS approximations are shown, in the energy region measured, along with the experimental points. From this comparison we find rather good agreement between theory (HF) and experiment, although this could be misleading as the measurement provides only a *relative* cross section.

Another method to locate the zero in the $6d \rightarrow \epsilon f$ dipole matrix element is through looking at the photoelectron angular-distribution asymmetry parameter β. General considerations[11] show that when the $6d \rightarrow \epsilon f$ dipole matrix element vanishes, $\beta = 0.2$. (Note, however, that a $\beta = 0.2$ does not necessarily imply a zero.) Turning to Fig. 4, which shows the β's for the various approximations, it is seen that the zero is located at $\epsilon = 0.13$ Ry for the HS calculation, and 0.93 and 0.95 Ry for the HF length and velocity, respectively. Furthermore, the resonancelike behavior of β is very pronounced and should be measurable over a fairly broad region, from about 0.8 to 1.2 Ry.

In conclusion, then, we find that the measurement appears to be in good agreement with our HF results and that the HS approximation predicts a minimum at much too low an energy. It is also pointed out that it might be easier to look at the photoelectron angular distribution to determine the existence and location of the minimum. Finally, we note that our HF results are entirely consistent with those of another recent calculation[4] which considered other excited d states in Cs using both HF and random-phase approximation calculations.

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