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Photoionization of the excited Cs 5*d* state

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Calculations of the photoionization cross section of the excited 5*d* state of atomic Cs are performed and found to be in excellent agreement with a recent absolute experiment [M. A. Bouchiat, J. Guena, Ph. Jacquier, and M. Lintz, Chem. Phys. Lett. **199**, 85 (1992); M. A. Bouchiat, C. Bouchiat, J. Guena, Ph. Jacquier, and M. Lintz, Z. Phys. D (to be published)].

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The photoionization of excited states of atoms has been of increasing interest recently as experimental techniques for producing and photoionizing even nonmetastable states have improved [1–3]. In addition, photoionization of excited states is of great importance in stellar opacities and in any other environment hot enough to produce them in quantity, along with the inverse process of radiative recombination. Theory has made a variety of predictions of new phenomenology for excited-state photoionization [4–9], predictions which have not yet been tested experimentally. A number of these predictions have involved excited *d* states of Cs. It is thus of great interest

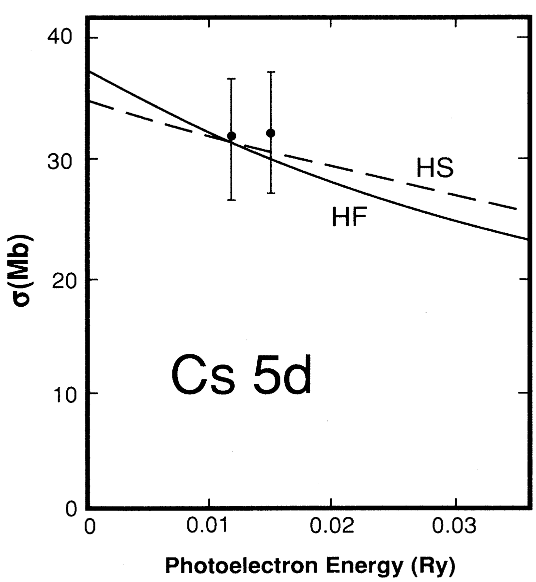

FIG. 1. Photoionization cross section for Cs 5*d* in Mb (10^{-18} cm^{-2}) as a function of photoelectron energy in Ry (13.6 eV). The points are the experimental results of Refs. [8,9], the solid curve is the Hartree-Fock (HF) result, and the dashed curve is the central-field Hartree-Slater (HS) cross section. The HF threshold energy, which differs very slightly from experiment, was used to put the experimental points on a photoelectron energy scale.

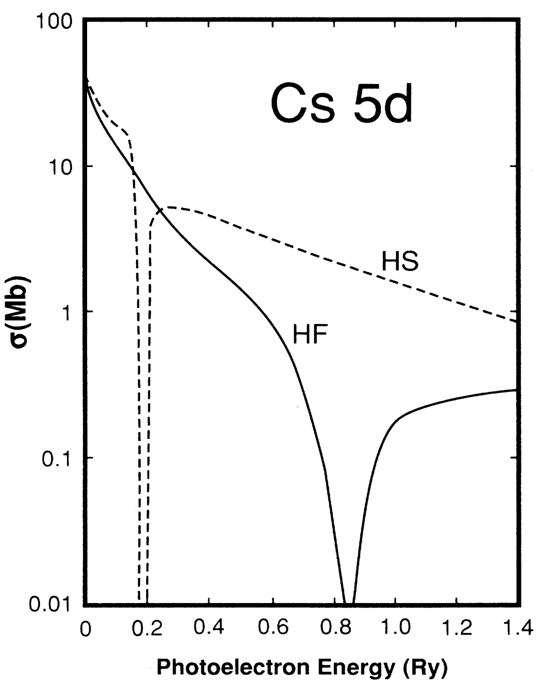

FIG. 2. Photoionization cross section for Cs 5*d* in Mb (10^{-18} cm^2) as a function of photoelectron energy in Ry (13.6 eV). The solid curve is the Hartree-Fock (HF) result and the dashed curve is the central-field Hartree-Slater (HS) cross section.

to test these predictions experimentally. Even if the predictions are not tested directly, however, any comparison of theory and experiment for photoionization of excited d states in Cs gives us information about the utility of the wave functions employed and thus indirect evidence concerning the predictions of new phenomenology.

Recently, an absolute measurement has been made of the photoionization cross section of the $5d$ excited state of Cs at two energies near threshold [10,11]. To use this to assess the accuracy of theory, we have performed Hartree-Fock (HF) calculations, including core relaxation [12,13], for the Cs $5d$ state which have been found to be good for Cs $7d$ photoionization [14]. A comparison of the results is shown in Fig. 1, where it is seen that the calculated HF cross section lies well inside the experimental error bars. The HF calculation was done in both length and velocity formulations [13,15], but they are so closely in agreement that only a single HF curve is shown in Fig. 1. Note that both the theory and the experiment are absolute with no adjustable parameters, making the agreement particularly meaningful. Note also that the HF result is in substantial, but not complete, agreement with the unrelaxed HF of Ref. [7].

Also shown in Fig. 1 is the result of a simple central-field Hartree-Slater (HS) calculation [16,17]; this cross section is based on the potential appropriate to the excited initial state, but this result is in close agreement with an earlier HS result [4] based on the ground-state potential. This HS cross section is also in good agreement with the experiment and with the HF result in the threshold region as shown in Fig. 1. This agreement, however, is due to the specific energy region in which the measurements were made. Looked at over a broader energy range, as shown in Fig. 2, the HF and HS cross sections are quite dissimilar quantitatively; the details and origin of these differences were discussed earlier in connection with Cs $7d$ photoionization [14]. Briefly, the dominant transition is $5d \rightarrow \epsilon f$ and the f-wave potential is double welled with a barrier between. In the HS calculation, the barrier is too low, which makes the ϵf move in at too low an energy, giving the low energy minimum shown in Fig. 2, and too broad, which causes the ϵf to remain outside until it reaches the top of the barrier, and then to move in very rapidly, giving the very sharp minimum seen in Fig. 2. In any case, while both calculations show a minimum which dominates the oscillator strength distribution over a significant region of the spectrum they are quantitatively *very* different in the region shown in Fig. 2 *except* just at threshold, below the minima. Actually, the results of HF and HS calculations again converge at higher energies (now shown) well above the minima. Thus, away from the minima, the HS formulation is not bad, a conclusion borne out by the recent experiment.

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