Photoelectron angular distribution of the excited $2p^2 3p$ ^2S state of atomic nitrogen

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Calculations of the photoelectron angular distribution asymmetry parameter β for the excited $2p^2 3p$ ^2S state of atomic nitrogen have been performed using Hartree-Fock discrete and continuum wave functions with relaxation. The results show reasonably good agreement with a recent measurement of β at a single energy.

I. INTRODUCTION

The photoionization of excited states of atoms is a process of importance in a number of connections, along with its inverse process, radiative recombination. In addition, there is great interest in this process at a fundamental level owing to the rich phenomenology associated with the absorption of photons by the physically large, excited atoms;[1−3] phenomenology which differs markedly from ground states. Unfortunately, due to various technical problems associated with the production of excited-state targets in the laboratory, there is not much in the way of experimental measurements of excited-state photoionization cross sections.

In addition to photoionization cross sections, which give information about absolute squares of transition-matrix elements (dipole-matrix elements for low photon energies[4]), photoelectron angular distribution asymmetry parameter β gives information on the matrix elements themselves, along with their relative phases.[5] One such measurement of β has recently been reported for the excited $2p^2 3p$ ^2S state of atomic nitrogen.[6] Some calculations of the β have been performed,[7,8] but only at the central-field level from which term-dependent effects are absent. Thus, while such calculations could be expected to explain the behavior qualitatively, detailed quantitative understanding can come only from a theoretical framework that includes exchange correctly, i.e., term dependence, explicitly; the Hartree-Fock (HF) calculation is the simplest such framework.[9] This is of importance because recent experience has shown that the photoionization is very strongly a function of the particular LS term of the initial state.[10]

We have thus performed HF calculations for the photoionization of the $2p^2 3p$ ^2S state of atomic nitrogen. In Sec. II, a brief review of the HF calculation is given. Section III presents and discusses our results for the cross section and asymmetry parameter. Section IV presents a summary and some final remarks.

II. BRIEF REVIEW OF THEORY

Within the framework of the electron dipole approximation, which is excellent for low-energy photons,[11] the photoionization cross section for a single electron in a subshell takes a fairly simple form.[12] In particular, for a transition $(L_c S_c nl)LS \rightarrow (L_c S_c \epsilon l')L'S$, an initial nl electron coupled to a core $L_c S_c$ to give LS going to a final continuum $\epsilon l'$ coupled to a core $L_c S_c$ giving $L'S$, the cross section is given by[12]

$$\sigma_{nl}^{L_c S_c L}(\epsilon) = \frac{4\pi \alpha a_0^2}{3}(\epsilon + I)$$

$$\times \sum_{l',L'} (2L'+1) l_> \begin{Bmatrix} l & L & L_c \\ L' & l' & 1 \end{Bmatrix}^2$$

$$\times M_{nl,\epsilon l'}^{L_c S_c LL'^2} , \tag{1}$$

where I is the ionization potential of the nl in the particular state, a_0 is the Bohr radius, α is the fine-structure constant, $l_>$ is the maximum of l and l', $\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix}$ is the Wigner 6-j symbol,[13] and

$$M_{nl,\epsilon l'}^{L_c S_c LL'} = \int P_{nl}^{L_c S_c L}(r) r P_{\epsilon l'}^{L_c S_c L'} dr , \tag{2}$$

where the P's are (r times) the radial wave functions for initial and final states of the electron undergoing the transition. The initial discrete wave function was obtained from a standard code,[14] while the final continuum wave function in the field of the fully relaxed ion was obtained from our own code.[15]

Using the matrix elements and phase shifts, the photoelectron angular distribution parameter β was calculated using the angular momentum transfer formulation,[16] which is described in detail elsewhere.[5] The calculation was performed in both the length formulation, Eq. (2), and the velocity formulation of the matrix element in an attempt to assess accuracy.

III. RESULTS AND DISCUSSION

Calculations have been carried out in the near-threshold region for the N $2p^2 3p$ ^2S photoionization channels. Before presenting the results, however, it is worthwhile to point out some general features of excited-state photoionization. The occurrence of Cooper minima[17] (zeros in dipole-matrix elements) has been found to be governed by the relative phase-shift (quantum-defect) difference between initial discrete and final continuum states at threshold. The continuum phase shifts for both s and d waves are almost exactly the same, in our calcula-

tions, for Hartree-Slater (HS) and HF. The initial discrete-state binding energies are −0.1869 and −0.2080 Ry for HS and HF, respectively, leading to quantum defects of 0.69 and 0.81, however, the latter being in rather good agreement with the experimental value of 0.85. In both cases the d-wave phase shift at threshold is about 0.01 (in units of π), so that the threshold phase-shift differences are 0.68 and 0.80 in HS and HF, respectively, for the $p \rightarrow d$ transitions.

Two specific facts known about the relation of the Cooper minima to the phase-shift differences[2,3] are that the difference must be at least about 0.5 to have a zero and the larger the difference, the higher the energy at which the zero appears. Our results for this case confirm these relations, as seen in Fig. 1 where the HS and HF $3p \rightarrow \epsilon d$ cross sections are shown. From these cross sections it is clear that the HS Cooper minimum occurs much closer to threshold than the HF length and velocity minima, just as the threshold phase-shift differences predicted. Furthermore, the HS phase difference, being just a bit above 0.5, is quite close to threshold; the HF are much further above threshold, having a significantly larger phase difference.

For the $3p \rightarrow \epsilon s$ transitions, the matrix elements and cross sections are determined by the inside, rather than the outer, region since the s-wave is so penetrating. Thus, despite the difference in quantum defects between HS and HF discrete states, the $3p \rightarrow \epsilon s$ cross sections are rather similar.

Note further that the HF length and velocity results are quite close to each other. This indicates that HF is likely to be an adequate description of the process. The zero in the length formation is slightly higher in energy than the velocity zero. The importance of the location of the $p \rightarrow d$ zero is that the photoelectron angular distribution asymmetry parameter β *must* have a value of zero at such a Cooper minimum.[18]

In any case, it is important to emphasize that β depends upon the $p \rightarrow s$ and $p \rightarrow d$ dipole-matrix elements, along with the relative phase shift between them. In particular, the expression is particularly simple in this case and is given as[5]

$$\beta = 2 \frac{R^2 - 2R \cos\Delta}{1 + 2R^2} , \tag{3}$$

where R is the ratio of the $p \rightarrow d$ to $p \rightarrow s$ matrix elements and Δ is the phase-shift difference (including the Coulomb phase). As discussed above, it is only the $p \rightarrow d$ matrix element that differs for HS and HF, the $p \rightarrow s$ and Δ are more or less unchanged.

The results of the β calculation are shown in Fig. 2 along with the experimental result of Ref. 6 and the HS result.[8] The agreement between experiment and the HF results (particularly velocity) is reasonably good, and the HF β's agree quite well with each other. The HS result, on the other hand, is in poorer agreement with experiment, and its shape in the low-energy region differs markedly from the HF result. This is due to the location of the Cooper minimum, which occurs at much lower energy for HS and HF, as detailed above. Thus the HF calculation shifts the HS β up and to higher energies, bringing it into better, but not perfect, agreement with experiment.

At this point it is worthwhile to consider the various aspects of correlation omitted from the calculation, and what effects these omissions are likely to have. Principal among the aspects of correlation omitted are the interchannel interactions in the final state of the ion plus photoelectron system, notably interactions with the $2p^2 3p \rightarrow 2p^2 \epsilon l'$ ($l' = d,s$) terms. While these channels are closed in the energy region of the measurement, they can still be mixed with the $2p^2 3p \rightarrow 2p^2 \epsilon l'$ channels, albeit with a small coefficient. Since the dominant $2p \rightarrow \epsilon d$ channel has no Cooper minima, i.e., the matrix element is positive, a small admixture with a $3p \rightarrow \epsilon d$ channel would make the latter matrix element somewhat more positive, moving the Cooper minimum closer to threshold and the dip in β to slightly lower energy; this would bring β into
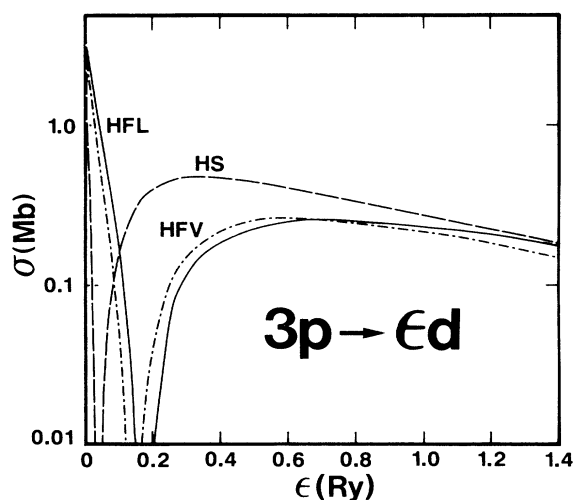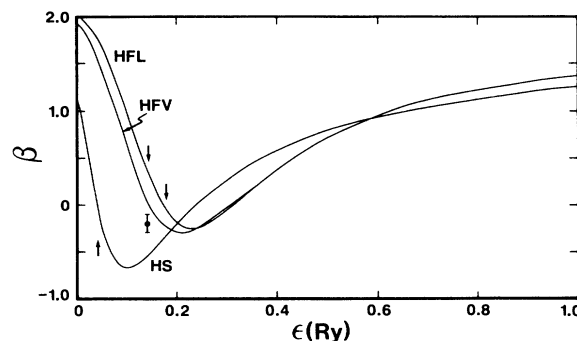

FIG. 1. Partial cross section for the Hartree-Fock length (HFL) and velocity (HFV) $2p^2 3p\, ^2S \rightarrow (2p^2 3p\epsilon d)^2P$ photoionizing transition, along with the Hartree-Slater $3p \rightarrow \epsilon d$ result of Ref. 8.

FIG. 2. Photoelectron angular distribution asymmetry parameter β for the HFL and HFV $2p^2 3p\, ^2S \rightarrow (2p^2 3p\epsilon d)^2P$ photoionizing transition, along with the (HS) $3p \rightarrow \epsilon d$ result of Ref. 8. The arrows, where each β is zero, indicate the position of the Cooper minimum in each case. The experimental point is from Ref. 6.

much better agreement with experiment as can be inferred from Fig. 2. Thus, in going from HS to HF, exchange effects move the Cooper minimum out, but it seems to "overshoot" the mark; interchannel coupling would have the effect of moving the minimum back in slightly towards threshold.

IV. FINAL REMARKS

In this paper it has been shown that the HF methodology gives satisfactory agreement of theory with experiment for the $2p^2 3p$ ^2S photoelectron angular distribution. The possible role of interchannel coupling was also discussed and the case was made for how it would likely bring theory and experiment into better agreement. In addition, the relationship between phase-shift differences and excited-state Cooper minima, verified previously only for HS calculations, has been shown to obtain in a HF case.

Finally, we note that the ^2S state is but one of the manifold of ten LS $2p^2 3p$ states. It is of great interest to inquire as to how the photoionization of each of these states differs, as a measure of the effectiveness of exchange interactions; such a calculation is in progress.

ACKNOWLEDGMENTS

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