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INNER SHELL PHOTODETACHMENT OF Na^- USING THE MULTI-CONFIGURATION TAMM-DANCOFF APPROXIMATION

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Abstract. The multi-configuration Tamm-Dancoff approximation (MCTD) is used to calculate the inner shell photodetachment of the Na anion. The results reproduce a resonance peak in agreement with existing experimental and theoretical data. The current work emphasizes the importance of doing configuration interaction (CI) type calculations, and proves MCTD is an apt tool to investigate the photoionization/photodetachment process.

1. INTRODUCTION

There have been many theoretical and experimental works investigating the photodetachment of negative ions as the photodetachment parameters are mainly governed by many-electron correlations (Ivanov 1999, 2004). Among the many successful theoretical methods applied to investigate photoionization/photodetachment process, some of them are the close-coupling method (Moores and Norcross 1974), R-Matrix (Rambsbottom et al. 1993, 1994), K-Matrix-L^2 (Moccia and Spizzo 1990), random phase approximation (RPA) (Chang and Fano 1976, Amusia et al. 2005), relativistic random phase approximation (RRPA) (Johnson and Lin 1979, Johnson et al. 1980, Radojević et al. 1987), RRPA with relaxation (RRPA-R) (Radojević et al. 1989, Kutzner et al. 2003), many-body perturbation methods (Chase and Kelly 1972), multi-configuration Hartree-Fock/Dirac-Fock (MCHF/MCDF) techniques (Froese Fischer and Hansen 1991), etc. Recently RRPA method was employed to investigate the interchannel coupling effect on the non-dipole photodetachment parameters of Cl^- **(**Jose et al. 2009). Besides valence shell photodetachment, the inner/intermediate shell photodetachment process is also of key significance because of several reasons. Inner shell photodetachment is usually followed by Auger decay and, thereby, the inner shell photodetachment process stands out as an excellent probe for post-collision interactions (Covington et al. 2007, Zhou et al. 2001, Berrah et al. 2001, Gorczyca 2004, Covington et al. 2001, Ivanov and Yatsyshin 2009). Inner/intermediate shell photodetachment can

lead to dramatic relaxation of outer electrons also. The RRPA-R method was successfully applied recently to investigate the near threshold relaxation effect of intermediate shell photodetachment of Cl^- and Br^- (Radojević et al. 2009). In the present work, inner shell photodetachment of of Na^- (2p) is investigated using the multiconfiguration Tamm-Dancoff approximation (MCTD) (Radojević and Johnson 1985), which includes relativistic effects and effects of many-electron correlations.

2. BRIEF DISCUSSION OF THEORY AND METHOD OF CALCULATION

In MCTD, final state correlations are included *via* time forward (positive frequency) Feynman-Goldstone diagrams while initial state correlations are included by adopting a multiconfiguration wavefunction in the initial state (Radojević and Johnson 1985). Since negative ions are highly correlated systems and can have doubly excited states, we have employed the multi-configuration Tamm-Dancoff (MCTD) approximation which can, in fact, account for such states to treat photodetachment of negative ions. In our MCTD calculation, the following six configurations have been used to represent the ground state of Na^-:

$$1s^2 2s^2 2p^6 (3s^2 + 3p_{1/2}^2 + 3p_{3/2}^2 + 3d_{3/2}^2 + 3d_{5/2}^2 + 4s^2),\ J=0.$$

For our calculation, the GRASP92 (Parpia et al. 1996) package is used to obtain multiconfiguration Dirac-Fock (MCDF) wavefunctions and configuration weights, which is an improved version of the Oxford multi-configuration Dirac-Fock (MCDF) code by Grant et al. (1980). The threshold for detachment of the i^{th} subshell (I_i) is obtained as $I_i = (E_N - E_{N-1})$, where E_N is the total energy of the negative ion in the ground state and E_{N-1} is the total energy of the neutral atom (N-1 electron system) in which a hole is placed in the i^{th} subshell. To calculate the excited state wavefucntion, all the allowed dipole transitions from the subshells 3s, 3p and 2p are taken into account for Na^-. The results of the calculations of inner shell photodetachment of Na^- are given in the next section.

3. RESULTS AND DISCUSSION

As mentioned in the introduction, the inner/intermediate shell photodetachment process is significant as the photodetachment can be followed by Auger decay and result in the formation of a positive ion (Covington et al. 2007, Zhou et al. 2001, Berrah et al. 2001, Gorczyca 2004, Covington et al. 2001, Ivanov and Yatsyshin 2009). There have been some experimental and theoretical efforts towards the inner shell photodetachment of Na^- (Covington et al. 2001, Ivanov and Yatsyshin 2009). We have calculated the photodetachment parameters of the 2p subshell of Na^-. The experimental cross section for photodetachment of the negative ion leading to a positive ion *via* Auger decay is compared with single photodetachment cross section from our MCTD results, since virtually every photodetachment process leads to positive ion production *via* Auger decay (Berrah et al. 2001).

The calculated total photodetachment cross section above the 2p threshold of Na^- is shown in Fig. 1. The major contribution to the total cross section comes from the 2p subshell. Experimental results (Covington et al. 2001) show resonance behavior of cross section at the 2p threshold, denoted as resonance (1), which GRPAE (with polarization) (Ivanov and Yatsyshin 2009) reproduces very well, but MCTD could not. The reason for the resonance (1) structure is the polarization effect and the absence of any polarization effect in MCTD is likely the reason why the MCTD result does not show sharp resonance behavior near the 2p threshold. The experimental result shows a broad resonance (2) in the region of photoelectron energy between 0.092 a.u. and 0.13 a.u., which is reproduced well by MCTD, but at a slightly different energy. The resonance structure (2) might be due to autoionizing transitions to the excited $2p_{1/2}^2 2p_{3/2}^3 3s^1 3p_{3/2}^2$ and $2p_{1/2}^1 2p_{3/2}^4 3s^1 3p_{3/2}^2$ of Na^- as also suggested by the experimentalists. GRPAE does not reproduce this structure well since it is a single configuration result and omits the kind of configuration interaction included in MCTD. GRPAE also overestimates the cross section in the higher energy region; the present MCTD result is in better agreement with experimental results at the higher energies. Neither calculation show the very narrow resonance 3, which must arise from a configuration interaction effect not included in either calculation.

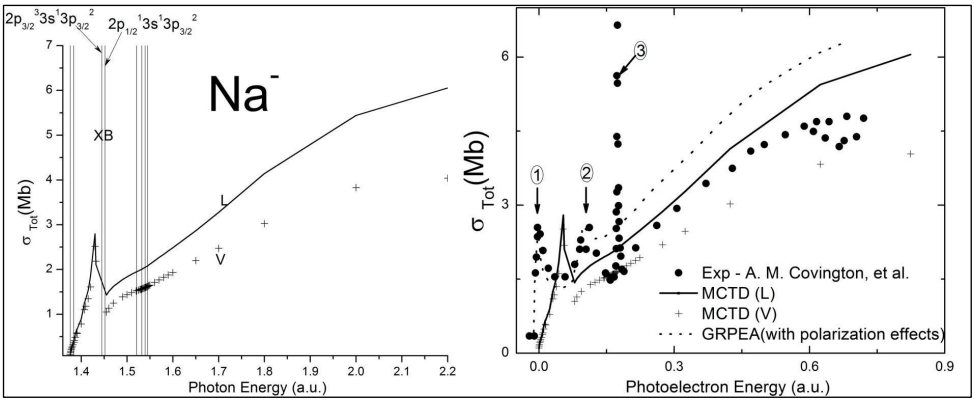

Figure 1. Inner shell photodetachment cross section of Na^- in length (L) and velocity (V) formulations. In the left panel, XB refers to excited bound states of Na^-. The MCTD results are compared with experimental (Covington et al. 2001) and other theoretical results (Ivanov and Yatsyshin 2009) in the right panel of the figure. The unlabelled vertical solid lines correspond to the thresholds for channels leading to: (*i*) $2p_{1/2}^2 2p_{3/2}^3 3s^2$, (*ii*) $2p_{1/2}^1 2p_{3/2}^4 3s^2$, (*iii*) $2p_{1/2}^2 2p_{3/2}^3 3p_{1/2}^2$, (*iv*) $2p_{1/2}^1 2p_{3/2}^4 3p_{1/2}^2$, (*v*) $2p_{1/2}^2 2p_{3/2}^3 3p_{3/2}^2$, (*vi*) $2p_{1/2}^1 2p_{3/2}^4 3p_{3/2}^2$ (in order from left to right).

In short, we have investigated the inner shell photodetachment of Na^- and the results are qualitatively in good agreement with other experimental and theoretical results. It is to be stated that the photodetachment parameters of negative ions have signature of many electron correlation effects; thus the importance of a configuration interaction calculation is evident.

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