Publ. Astron. Obs. Belgrade No. 84 (2008), 61 - 64 *Contributed Paper*

PHOTODETACHMENT OF 2p SHELL OF THE CHLORINE NEGATIVE ION

V. RADOJEVIĆ[1], J. JOSE[2], G. B. PRADHAN[2], P. C. DESHMUKH[2] and S. T. MANSON[3]
[1]*Institute of Physics, P. O. Box 57, 11001 Belgrade, Serbia*
E–mail: vradoje@phy.bg.ac.yu
[2]*Department of Physics, Indian Institute of Technology - Madras, Chennai 600 036, India*
E–mail: pcd@physics.iitm.ac.in
[3]*Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303, U. S. A.*
E–mail: smanson@gsu.edu

Abstract. The photodetachment cross sections are calculated for intermediate, $2p$ shell of the chlorine negative ion in the relativistic random-phase approximation (RRPA) to account for relativistic effects and many electron correlations, and in modified RRPA (RRPA-R) to additionally account for relaxation of atomic core in the photodetachment process. The results of calculations with and without relaxation effects are compared.

1. INTRODUCTION

There has been relatively recently rapid development in the physics of negative ions, particularly in investigations of many body effects in electron structure and photodetachment process (Ivanov, 1999, 2004, and references therein). One of the approaches that has been rather successful in describing the photoionization process of neutral atoms and positive ions, and that takes into account the many-electron correlations, is the random-phase approximation (RPA) in nonrelativistic form (usually refered to as RPAE) (Amusia and Cherepkov, 1975, Wendin, 1976) and and its relativistic version (RRPA) (Johnson and Lin, 1979, Johnson et al. 1980). The RRPA has been applied to photodetachment of negative halogen ions (Radojević et al. 1987) and the agreement with a limited amount of experimental data available has been quite reasonable.

However, the RPA (whether it is RPAE or RRPA) does not include the effects of a relaxation of remaining atomic core in the photoionization process. It has been demonstrated that by applying modified RPAE to include relaxation effects (GRPAE) (Amusia et al. 1976) as well as modified RRPA (RRPA-R) (Radojević et al. 1989) that these effects are significant for some inner shells of neutral atoms and mostly in an energy region close to the ionization threshold of the considered shell. The RRPA-R has been also applied to photodetachment of outer shells of I^- (Z=53) (Radojević, 1992), Br^- (Z=35) (Altun and Radojević, 1992), F^- (Z=9) and Br^- (Z=35) (Robertson, et al. 2000), and Cl^- (Z=17) (Kutzner et al. 2000).

There were until recently few calculations of the inner-shell photodetachment from negative ions (Ivanov 2004), and the applications of the RRPA and RRPA-R were mostly done for photodetachment of valence shells. In a few applications of RRPA and RRPA-R to photodetachment of valence shells of negative ions, some intermediate shells were treated, like I^- 4d (Radojević and Kelly, 1992) and Br^- 3d (Altun and Radojević, 1992).

In the present study the RRPA and RRPA-R are applied to the photodetachment of the inner $2p$ shell of Cl^-. Unfortunately, there are no experimental data known to us for the processes treated in the present work, with which we could compare our results.

2. METHODS AND CALCULATIONS

Dipole excitations from the $3p$, $3s$, $2p$, and $2s$ shells have been included in our calculations, thereby producing 14 jj-coupled channels. The channels arising from the excitations of the innermost $1s$ shell have been omitted (truncated RRPA) as there is very small interaction (coupling) of this shells with those included. We performed some calculations with inclusion of the channels arising from excitation of the $1s$ shell, and the results are practically the same as without its inclusion.

The relaxation effects were included in RRPA-R by performing the RRPA-type calculations and computing the excited-state orbitals in the field of self-consistently calculated orbitals for relaxed neutral atom (V^{N-1} potential), i.e. the neutral atom with the hole in the shell which is the origin of a given channel.

In our study of the photodetachment of the $2p$ shell the hole state of the relaxed atom may be placed either in the $np_{3/2}$ or in $np_{1/2}$ subshell. We have chosen to place it in the $np_{3/2}$ subshell since it has a lower ionization energy and has the greater degeneracy. It was found in some earlier calculations (Radojević et al. 1989, Kutzner et al. 1989) that the results depend weakly on which subshell is chosen.

Overlaps between orbitals of the relaxed atom and those of the ground state of negative ion multiply the dipole matrix elements (Radojević et al. 1989) in the RRPA-R calculations and this leads to the reduction in the np cross section by approximately 20% for. The theoretical values of the channel thresholds in the strict RRPA are the absolute values of the Dirac-Hartree-Fock eigenvalues. In the relaxed-core calculations, the differences between the total energies calculated self-consistently for the relaxed neutral atom with a hole in a considered subshell and the ground state of the negative ion (ΔE_{SCF} values) are used for the thresholds. The relevant calculated threshold energies are presented in Table 1.

Table 1: The photodetachment thresholds of Cl^- in a.u. used in present work. Presented are Dirac-Hartree-Fock values (DHF) used in RRPA and ΔE_{SCF} values used in RRPA-R calculations.

Subshell	DHF	ΔE_{SCF}
$3p_{3/2}$	0.1480	0.0927
$3p_{1/2}$	0.1532	0.0969
$3s_{1/2}$	0.7398	0.6660
$2p_{3/2}$	7.6762	7.2214
$2p_{1/2}$	7.7410	7.2832
$2s_{1/2}$	10.2981	9.8776

The threshold energies, as well as all the orbitals used in present work were calculated using the Oxford multiconfiguration Dirac-Fock package by Grant et al. (1980). These orbitals and energies could be calculated using any other, even single configuration Dirac-Fock code, and interfacing the RRPA-R code appropriately.

3. RESULTS

The results of our RRPA and RRPA-R calculations for partial cross sections are shown in Fig. 1. The length and velocity form results in our (truncated) RRPA practically coincide in our calculations. All calculated partial cross sections vanish (or seems to vanish) at the corresponding threshold, satisfying (or showing the tendency) to satisfy the Wigner threshold law for negative ions (Wigner 1948), according to which the cross section vanish at the corresponding threshold. Let us note that the RRPA and RRPA-R codes cannot run at the very threshold. Each partial cross section increases with increase of the photon energy in the very vicinity of its threshold, then reaches a maximum relatively close to the threshold, and at higher energies decreases monotonically. One notices a big difference between both types of calculations (RRPA and RRPA-R) in the region of energies around the corresponding maximum of the cross section and in the vicinity of the threshold. This difference cannot be completely ascribed to the reduction of transition matrix elements when relaxation of atomic core is taken into account in the RRPA-R calculations.

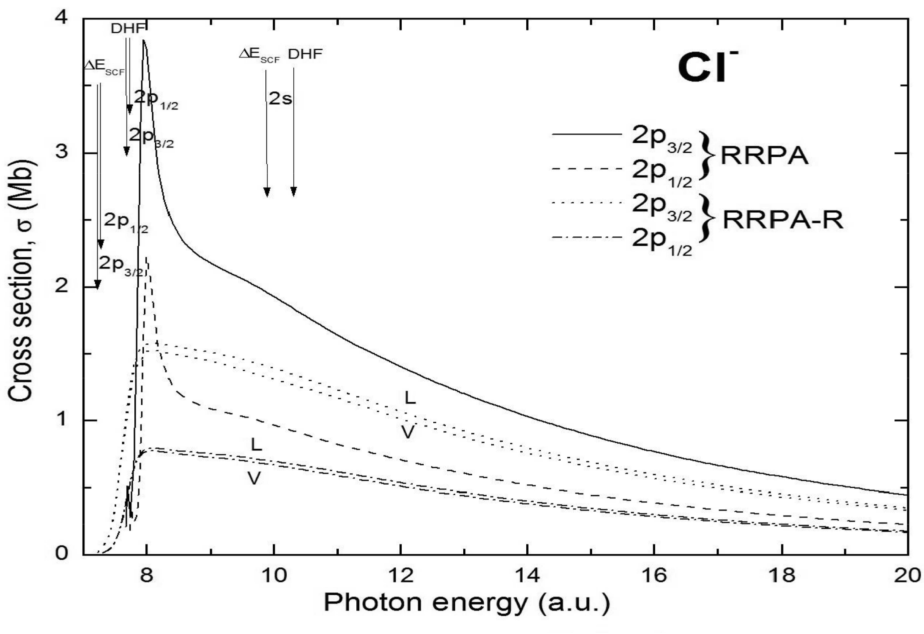

Figure 1: Photodetachment partial cross sections of Cl^{-} $2p$ shell in RRPA and RRPA-R.

4. CONCLUDING REMARKS

In our present calculations, relativistic effects and significant interchannel correlations are included. Furthermore, in the RRPA-R calculations are included the effects of relaxation of the atomic core in the photodetachment process. Through the inclusion of the overlaps, transfers of the oscillator strengths from the main channels to doubly excited channels are approximately accounted (Kutzner et al 1989). However, it is assumed in our approach with the RRPA-R that the atomic core is fully relaxed during the photodetachment process, although relaxation is in general less than complete, and the degree of relaxation changes during the process. Perhaps the incomplete relaxation is responsible for the big difference between the RRPA and RRPA-R results, although all the reasons for this difference are not clear. It is already found in photoionization calculations that the RPA results close to the channel threshold are notably larger than the results with the relaxation effects included (Amusia et al. 1976, Radojević et al. 1989). Experimental data are extremely desirable to determine whether for the negative ions the results with relaxation effects included agree better than the results without, as has been found to be the case for photoionization of atoms (Amusia et al. 1976, Radojević et al. 1989).

Acknowledgments

This work was supported by a research grant from the Department of Science and Technology, Government of India. One of the authors (V.R.) wishes to acknowledge the hospitality extended by the Department of Physics at the Indian Institute of Technology -Madras, where the present work was carried out, and to the partial support of the Ministry of Science of the Republic of Serbia through the project No. 141029.

References

Altun, Z., Radojević, V.: 1992, *J. Phys B: At. Mol. Opt. Phys.*, **25**, 3757.
Amusia, M. Ya., Cherepkov, N. A.: 1975, *Case Stud. At. Phys.*, **5**, 47.
Amusia, M. Ya., Ivanov, V. K., Chernysheva, L. V.: 1976, *Phys. Let.*, **59A**, 191.
Grant, I. P., McKenzie, B. J., Norrington, P. H., Meyers, D. F., Pyper, N. C.: 1980, *Comput. Phys. Commun.*, **21**, 207.
Ivanov, V. K.: 1999, *J. Phys B: At. Mol. Opt. Phys.*, **32**, R6 7.
Ivanov, V. K.: 2004, *Rad. Phys. Chem.*, **70**, 345.
Johnson, W. R., Lin, C. D.: 1979, *Phys. Rev. A*, **20**, 964.
Johnson, W. R., Lin, C. D., Cheng, K. T., Lee., C. M.: 1980, *Phys. Scr.*, **21**, 409.
Kutzner, M., Radojević, V., Kelly, H. P.: 1989, *Phys. Rev. A*, **40**, 5052.
Kutzner, M., Robertson, J. A., Pelley, P.: 2000, *Phys. Rev. A*, **62**, 062717.
Radojević, V., Kelly, H. P., Johnson, W. R.: 1987, *Phys. Rev. A*, **35**, 2117.
Radojević, V., Kutzner, M., Kelly, H. P.: 1989, *Phys. Rev. A*, **40**, 727.
Radojević, V., Kelly, H. P.: 1992, *Phys. Rev. A*, **46**, 662.
Robertson, J. A., Kutzner, M., Pelley, P.: 2000, *Phys. Rev. A*, **63**, 042715.
Wendin, G.: 1976, In: Photoionization and Other Probes of Many-Electron Interactions, ed. F. J. Wuilleumier, p. 61, New York: Plenum.
Wigner, E. P.: 1948, *Phys. Rev.*, **73**, 1002.