CALCULATION OF AUTOIONIZING RESONANCES IN POSITIVE ION PHOTOABSORPTION

M1

V.K.Ivanov, A.N.Ipatov, A.A.Shavrin, M.S.Shendrik
St.Petersburg State Technical University, St.Petersburg 195251, Russia

In present report the results of theoretical study of resonance autoionizing structure in positive ion photoabsorption are presented. The concrete calculations of the partial and total photoionization cross sections and photoelectron angular distributions were performed within the methods based on the many-body theory. These methods use the Hartree-Fock approximation as the zero one and take into account the many-electron correlations within the Random Phase Approximation with Exchange (RPAE) for the calculations of phototransition amplitudes[1,2], the Dyson equation for the energy shifts (self-energy part) and corrections to wavefunctions of ground and discrete excited states, the many-body perturbation theory for the determination of Auger widths and relativistic corrections[3]. The photoionization cross sections and the shape resonance parameters have been calculated for the series of single and double charged positive ions.

The photoabsorption of outer 5s subshell of Sr^+ positive ion has been calculated both using the non-relativistic approximation and with account of relativistic corrections. The nonrelativistic calculations were performed within the Spin-Polarized version of the RPAE (the ground state Sr^+ structure of outer subshells is the following: $...4p^3\uparrow 4p^3\downarrow 5s\uparrow$) and with the self-energy corrections to resonance positions. The results of these calculations have revealed the strong autoionizing structure and the giant autoionizing resonance which may be attributed to the $4p \rightarrow 4d$ transitions. The similar strong resonance have been found in the 4s Ca^+ absorption spectrum[2] associated with $3p \rightarrow 3d$ transition.

The relativistic calculations are based on the using of the Dirac-Fock wavefunctions ($...4p^2_{1/2}\ 4p^4_{3/2}\ 5s_{1/2}$), and the many-electron correlations are taken into account within the relativistic version of the RPAE. These calculations of the Sr^+ photoabsorption spectrum are being completed at present and the results will be presented at the workshop.

The non-relativistic calculations have been performed for the autoionizing structure in 3p photoabsorption spectrum of K^+ and Ca^{+2} associated with $3s \rightarrow np$ excitations. The results of the calculations are very sensitive to the energy positions of these discrete excitations relatively the Cooper minimum in the partial $3p \rightarrow \varepsilon d$ cross section. Thus, the Hartree-Fock excitation energy for the $3s \rightarrow 4p$ transition in Ca^{+2} is equal to 59.7 eV and lies just nearby the Cooper minimum. For this transition one obtains the autoionizing resonance with Fano profile parameter $q \approx 40$ and width $\Gamma \approx 0.035$ eV, all next $3s \rightarrow 5p,6p,...$ resonances, lying above the Cooper minimum, have the negative values of q-parameter and smaller widths. Taking into account of the 3s-electron energy shift within the Dyson equation method the $3s \rightarrow 4p$ transition energy becomes equal to 54.4 eV. The calculation with this energy gives the q-parameter value $q \approx 4$ and width $\Gamma \approx 0.046$ eV. At present the calculations with the corrected energy and wavefunction for 4p excited state in Ca^{+2} are performed and the results also will be reported at the workshop.

1. M.Ya.Amusia, V.K.Dolmatov, V.K.Ivanov// Zh.Eksp.Teor.Fiz. 1983. v.85. p.115
2. V.K.Ivanov and J.B.West// J.Phys.B:At.Mol.Opt.Phys. 1993. v.26. p.2099
3. P.Dunne, G.O'Sullivan, V.K.Ivanov// Phys.Rev.A 1993. v.48. p.4358