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RESONANCE PHOTOABSORPTION OF ATOMS THROUGH THE AUTOIONIZATION DECAY OF THE DOUBLY-EXCITED STATES.

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1. Introduction

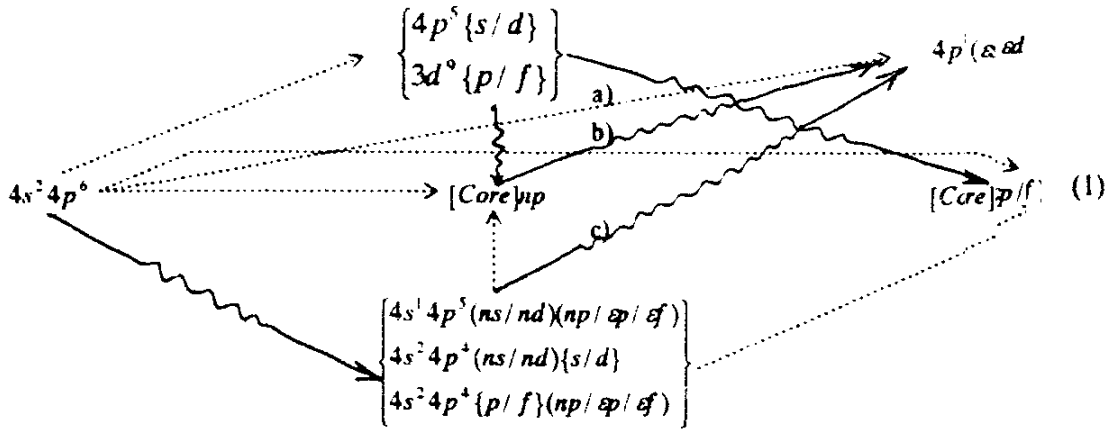
Study of the photoabsorption of the noble gas atoms in the photoionization threshold region of the subvalence shells is of special interest during last decades. This interest is connected with the fact that atomic photoionization in this energy range of incident radiation is almost entirely determined by many-electron effects. In particular,

- energy structure of the ionic states with the subvalence-shell vacancy is at great extent determined by the dipole polarization of the valence shells in the potential of the vacancy;
- the absolute values and the general shapes of the photoionization cross section spectra are determined mainly by the inter-shell correlations;
- the resonance structure of the photoabsorption spectra reflects the highly probable process of the atomic photoionization through the decay of the doubly-excited intermediate states.

In [1-7] (see also refs. therein) after the detailed theoretical and experimental study of the photoionization process the correlations discussed above were found to be dominating among a variety of many-electron processes. As a result, good agreement of measured and calculated values for many spectral characteristic have been obtained in those works. However, several disagreements still exist in [2-7] between theory and experiment. Thus, calculated absolute values of the photoionization cross sections for the satellite levels exceed respective experimental values approximately by a factor of 5. The main purpose of the present paper is to investigate the possible reasons of such a disagreement. The 4s- and 4p-photoabsorption spectra of the Kr atom have been used as an object of our study.

2. Technique of the calculations.

The technique of the calculation of the atomic wave functions and energies as well as that for the transition amplitudes have been described in detail in [2-7]. Therefore, in this paper only a principal scheme of our calculations is presented. The following processes have been considered in the calculations of the photoabsorption of the Kr atom:



Here broken lines denote the electric dipole interactions and the wavy line the Coulomb interactions of the electrons. The intermediate states $\{l\}$ were summed over the discrete spectrum states, nl, and integrated over the states of continuum, εl. The notation a/b means that either state a or state b is incorporated in the calculations of the transition amplitude according to the orthogonality conditions. The notation [Core] denotes the Kr II ionic states, which are the superposition of the single-configuration basis states.

The photoionization of the 4s-main line and the satellite levels of the Kr atom has been studied in [3-7]. In addition, the 4p-photoionization has been calculated in the present work since the photoionization through the decay of the doubly-excited states is expected to be reflected in this spectrum, too. The a), b), and c) amplitudes in scheme (1) describe the photoabsorption of the 4p-shell. The amplitude a) determines the direct photoionization, the amplitude c) - the intra-shell correlations, and the amplitude b) corresponds to the 4p-photoionization through the autoionization decay of the doubly-excited states.

3. Results and discussion.

The calculated photoionization cross sections of the 4s-main line and several satellite levels of the Kr atom are presented and compared with respective experimental values in fig. 1. The theoretical spectra have been calculated with accounting for the interference of the channels from scheme (1). For the convenient comparison of experimental and theoretical spectra, the calculated cross sections were convoluted with a Gaussian apparatus profile of the FWHM=10 meV. As one can see from the upper panel of fig. 1, in the 4s-main line spectrum, the doubly-excited states manifest themselves in all kinds of resonances: with window, profile and peak shapes. For the satellite levels, all the doubly-excited states are reflected as peak resonances. It makes it possible to compare the values of the oscillator strength integrated over the exciting photon energy. This value can be obtained using the following expression:

$$f(30.5)[a.u.] = \frac{1}{2\pi^2 \alpha a_0^2} \int_{threshold}^{\omega=30.5eV} \sigma(\omega)d\omega = \frac{1}{4.032} \int_{threshold}^{\omega=30.5eV} \sigma[Mb]d\omega \qquad (2)$$

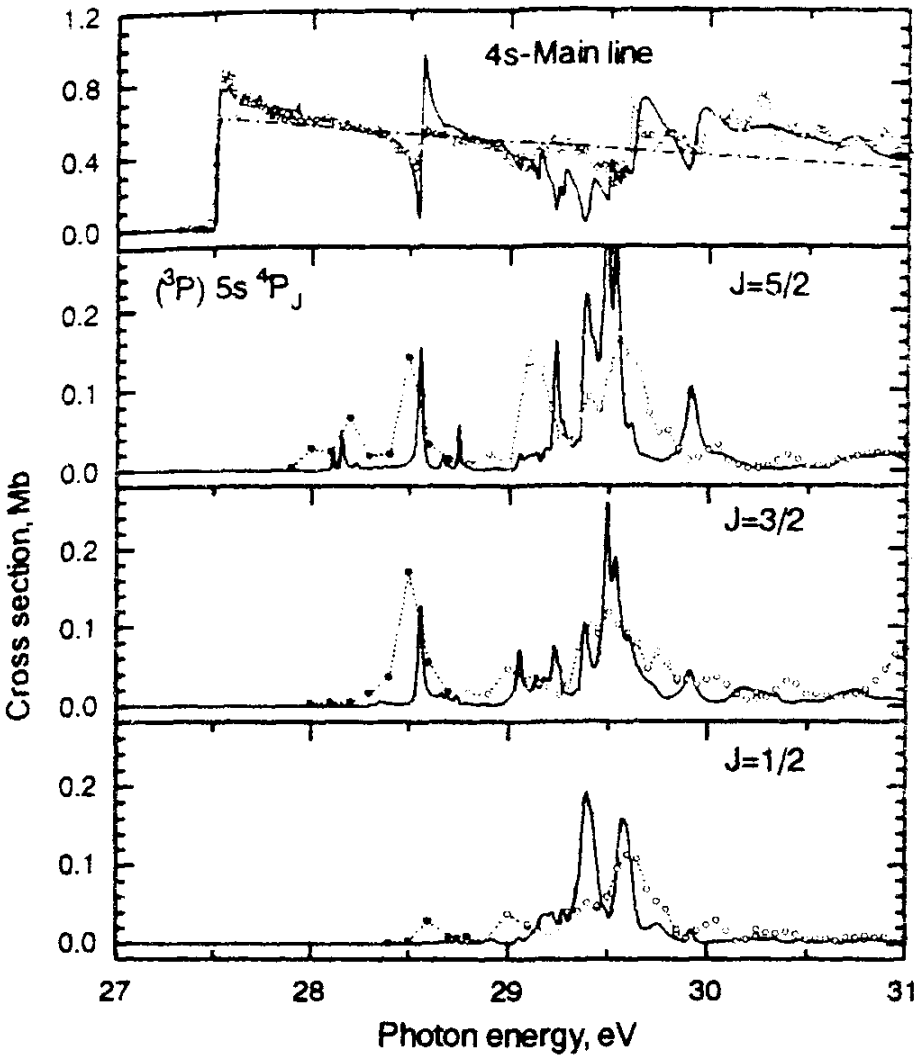


Fig.1 Measured and calculated cross sections of the 4s- Main and three satellite levels of the Kr atom. Solid line - theory reduced by a factor of 5; filled circles - experiment from [3]; open circles - experiment, present work; dash-dotted line - calculation without doubly- excited states .

Experimental and theoretical $f(30.5)$ values calculated using eq.(2), are presented in table 1. One see that the calculated oscillator strengths exceed experimental values approximately by a factor of n the same table, the results of the model calculations in which the transition amplitudes to the bly-excited states were reduced by a factor of 2.09, are also presented. In the latter case the oretical and experimental integrated oscillator strengths, $f(30.5)$, calculated using eq.(2), are in good cement for all the levels.

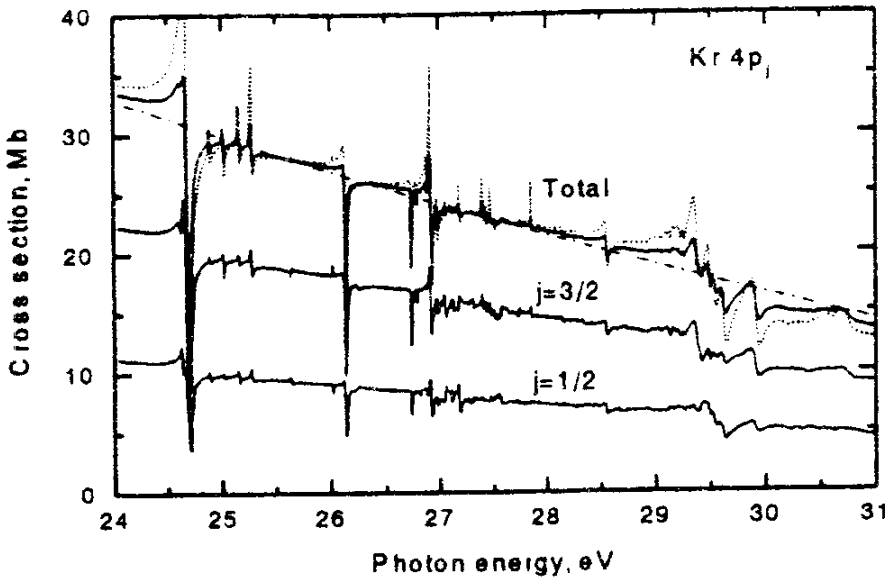


Fig.2 Total and partial cross sections of the 4p-shell calculated in two approximations: with (solid line) and without (dotted line) decrease of the transition amplitudes into the doubly-excited states. Dash-dotted line - calculation without the doubly- excited states.

Table 1. Calculated and measured energies and integrated oscillator strengths $f(30.5)$ (see eq.(2)). for the several low-lying satellite levels of the Kr atom.

Satellite state		*Energy, eV*		*Oscillator strength*		
		Theory	*Experiment* [8]	*Theory*	*Experiment*	*Model calculation*
$(^3P)\ 5s\ ^4P$	5/2	28.04	27.99	3.92	1.08	0.96
	3/2	28.30	28.27	2.89	0.93	0.96
	1/2	28.57	28.58	2.22	0.53	0.58
$(^3P)\ 5s\ ^2P$	3/2	28.69	28.69	2.77	0.74	1.14
	1/2	28.99	29.00	5.34*)	1.17	1.58
$(^3P)\ 4d\ ^4D$	7/2	28.92	28.90	1.11	–	0.26
	5/2	28.93	28.93	2.89	0.54	0.73
	3/2	29.03	29.00	5.34*)	1.17	1.58
	1/2	29.10	29.10	1.06	0.31	0.27
$(^3P)\ 4d\ ^4F$	9/2	29.62	29.62	0.29	–	0.06
	7/2	29.86	29.86	0.19	–	0.05
	5/2	30.05	30.08	0.18	0.08	0.05
	3/2	30.15	30.18	0.09	0.02	0.02

*) the sum for the $(^3P)5s\ ^2P_{1/2}$ and $(^3P)4d\ ^4D_{3/2}$ states is listed because of strong overlap of these states.

In order to study the changes in the theoretical 4p- photoabsorption spectrum of the Kr atom whicl can be caused by the reducing of transition amplitudes to the doubly-excited states, the two calculation have been performed as follows. In the first calculation the transition amplitudes were taken unchanged while in the second one they were reduced by a factor of 2.09. The results are presented in fig.2.

One can see that the spectrum obtained using the unchanged transition amplitudes to the doubly-excited states is dominated by the profile-type resonances, while the application of the reduced amplitudes gives mainly the window-type resonances. It is manifested the most impressively for the first resonance connected with the $4s^2 5p_{1/2}$ and $4s^2 5p_{3/2}$ doubly-excited states. Unfortunately, we have no precisely measured data on the 4p-photoionization cross sections for the Kr atom. However, so far as one can judge from the results of [9], the resonances in the 4p-photoabsorption spectrum are window-type ones.

In case the described above assumption about the shapes of the resonances in the 4p-spectrum is confirmed experimentally, and keeping in mind the existence of disagreements between the theoretical and experimental 4s-satellite spectra, one will be able to determine quite definitely the direction of the future theoretical investigations: the more precise calculations of the transition amplitudes to the doubly-excited states. Firstly, it will be necessary to take into account the rearrangement of the electron shells during the *excitation* process. This effect was not incorporated in our previous calculations [2-7] because of it's small influence on the theoretical *photoionization* cross sections of the valence atomic shells [1-3]. The additional experimental information can be obtained from the precise measurements of the 4p-spectrum in the photon energy region exceeding the 4s-ionization threshold ($\omega \sim 29$+30 eV). As one can see from fig.2, the deviations of the calculated cross sections from the monotonic curve in this range are quite sensitive to the values of the oscillator strengths of transitions to the doubly-excited states.

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