ARGON PHOTOIONIZATION IN THE REGION OF THE LOWEST RESONANCE OF THE TWO-PARTICLE–TWO-HOLE TYPE

S.I. STRAKHOVA and T.M. ZAYAC
Institute of Nuclear Physics, Moscow State University, Moscow 119899, USSR

Received 11 July 1984

The integral formulation of the close coupling method is used to calculate the cross sections of direct and resonance photoionization of Ar near the $3p^{-2}(^3P)4s4p\ ^1P$ resonance. The data obtained are compared with the experimental results and with calculations made elsewhere.

The spectrum of the quasistationary ^1P states of the Ar atom was studied experimentally in ref. [1]. Theoretical estimates of the Ar resonance parameters were obtained only for the lowest resonances of the particle–hole type by calculating the photoionization processes [2,3] and the cross sections of Ar ionization by electrons [4], as well as in the processes of electron scattering by ions [5]. The aim of this work is to calculate the two-particle–two-hole type lowest state profile in the cross sections of resonance photoionization of the Ar atom.

The lowest resonances of Ar are located against the background of direct transitions from the 3p-subshell to continuum. We have calculated the 3p-subshell contribution to the cross section of direct photoionization of Ar in a broad energy range. The Ar wave function above the ionization threshold was obtained by solving the set of two integral equations for the K-matrix:

$$K(\lambda, \lambda', \epsilon) + \sum_{\mu} \int_0^{\infty} \frac{\langle \lambda' \epsilon | \hat{V} | \mu \epsilon' \rangle}{\epsilon' - \epsilon_{\mu}} K(\lambda, \mu, \epsilon')\, d\epsilon'$$

$$= -\langle \lambda' \epsilon | \hat{V} | \lambda \epsilon_{\lambda} \rangle . \qquad (1)$$

Here $\epsilon_{\lambda} = E - E_{\lambda}$; E is the excitation energy of Ar; E_{λ} is the ionization potential of an atom in channel λ, $\hat{V}$ is the residual interaction ($\hat{V} = \hat{H} - \hat{H}_0$); $\hat{H}$ and $\hat{H}_0$ are the exact and model hamiltonians of Ar; $|\lambda\epsilon\rangle$ are basis functions in channel λ at energy ϵ which are eigenfunctions of the hamiltonian H_0. The sum includes two terms corresponding to the $3p^{-1}\epsilon s$ and $3p^{-1}\epsilon d$ channels. The integral is taken in the sense of the principal value. The expression for the continuum wave function, used to calculate the resonance photoionization cross section, includes the K-matrix in the following manner:

$$\Psi_{\lambda E} = \sum_{\mu} [1 - iK(\lambda, \mu, E)]^{-1}$$

$$\times \left(|\mu \epsilon_{\mu}\rangle + \sum_{\lambda'} \int_0^{\infty} \frac{K(\mu, \lambda', \epsilon)}{\epsilon - \epsilon_{\lambda'}} |\lambda' \epsilon\rangle\, d\epsilon \right) . \qquad (2)$$

The asymptotic of the basis functions $|\lambda\epsilon\rangle$ was chosen to be of the form of a standing wave; therefore, the expression (2) ensures the T-matrix asymptotic for the function $\Psi_{\lambda E}$. The calculations were made using the Hartree–Fock functions to describe the ground state of Ar. The basis functions $|\lambda\epsilon\rangle$ were calculated in the field of a frozen $3p^{-1}$ core. The cross sections of direct photoionization from the 3p-subshell are presented in fig. 1 which also shows, for comparison, the one-channel calculation results [6] and the experimental data [7]. The results of the calculation reproduce the cross section minimum arising from the shape resonance in the d-wave [6].

Resonance photoionization cross sections were calculated making allowance for close coupling of the two open channels mentioned above to two closed channels corresponding to the $3s^{-1}4p^1P$ and $3p^{-2}(^3P)4s4p^1P$ states, with the set of two integral

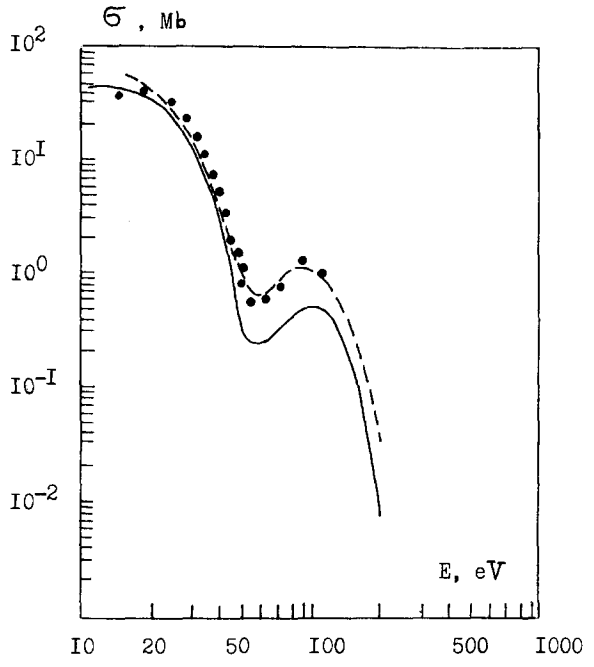

Fig. 1. The contribution of the 3p-subshell to the cross section of direct photoionization of Ar. The solid line shows the present calculations, the dotted line shows the experiment [7], the dashed line shows the calculations [6].

equations (1) being replaced by a set of four integro-algebraical equations with singular kernels. The set of such equations is given in ref. [8], which presents the results of the same calculations for Ne. *LS*-coupling was assumed to be valid for the classification of the states in the interval of the Ar excitation spectrum studied [5,9].

The basis functions in the subspace of closed channels were calculated with the Hartree–Fock approximation with complete selfconsistency, like the function of the Ar ground state, whereas the basis functions of the open channels were calculated in the frozen $3p^{-1}$ core. The results obtained are presented in table 1. We made use of the commonly adopted Fano designations for the resonance parameters [10].

From table 1 it is seen that the parameters of the two-particle–two-hole resonance in the version V of our calculations are in good agreement with experimental data. This result is insensitive to the replacement in the set of four integro-algebraical equations of the Hartree–Fock energy of this state by the experimental energy.

As to the $3s^{-1}4p$ state, the calculations [2,4] have shown that the parameters of this resonance calculated with the Hartree–Fock or Herman–Skillman one-configuration approximation, disregarding the decay channel coupling, are close to those obtained experimentally.

The calculations [2] have demonstrated a high model sensitivity of the $3s^{-1}4p$ parameters. In particular, this conclusion was drawn in ref. [2] from calculations in which the contribution of the two-particle–two-hole state was estimated but approximately. The conclusion has been confirmed by our calculations. Table 1 presents the results of our calculations in the cases when the experimental and

Table 1
The parameters of the lowest resonances in the cross sections of resonance photoionization of Ar.

State ^1P	Parameters	Present calculations		E_α^{exp}		E_α^{HF}		Experimental data [a]	Calculations made in			
		L	V	L	V	L	V		ref. [3]		ref. [2]	ref. [4]
									L	V		
$3p^{-2}(^3P)4s4p$	Γ, eV	0.026	0.013					0.02 ± 0.001				
	q	−0.5	−0.16					−0.2 ± 0.1				
	ρ^2	0.08	0.06					0.10 ± 0.02				
$3s^{-1}4p$	Γ, eV			0.04	0.04	0.04	0.04	0.080 ± 0.005	0.068	0.068	0.085	0.068
	q			−0.6	−0.66	−0.22	−0.20	−0.22 ± 0.05	−0.33	−0.29	−0.27	−0.33
	ρ^2			0.43	0.51	0.89	0.79	0.86 ± 0.04	0.855	0.86	0.89	0.86

[a] Ref. [1].

Hartree–Fock energies of states were used as the basis energies E_α in the set of four integro-algebraical equations.

The energy shifts of the states due to interconfigurational interactions prove to be insignificant.

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