DESCRIPTION OF SELF-IONIZATION STATES OF MULTICHARGE HELIUM-LIKE IONS IN THE INTERMEDIATE-COUPLING APPROXIMATION

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The diagonalization technique is employed for calculating the excitation energies and the widths of self-ionization $^1P_1^{(-)}$ and $^3P_1^{(-)}$ states of Fe^{24+} ions, converging to the n = 2 threshold of the residual ion. The calculations were performed with allowance for the spin-orbital interaction, and also in the LS coupling approximation. It is seen by comparing our results with calculations which included Breit's complete operator that in calculating the widths of self ionization levels of helium-like iron ions in the intermediate coupling approximation one can restrict himself to only the single-particle operator of the spin-orbital interaction. Here allowance for configuration mixing with respect to the principal quantum number results in only insignificant changes in the excitation energies and width of the self-ionization levels under study.

The effect of configuration superposition form the subject of many analytic studies of self-ionization states of two-electron systems. The majority of these studies is based on the diagonalization method [1], which is successfully employed in calculating the energy and widths of self-ionization states with atomic number $Z < 10$ [1,2], which makes allowance for the superposition of configuration in the coupling approximation. However, an increase in Z is accompanied by a rapid growth of the role of magnetic interactions, which significantly affect the structure of the self-ionization spectrum. In this case the description of self-ionization states must be constructed with simultaneous allowance for the electrostatic and magnetic interactions. The scale of the expected effects can be easily estimated by means of the intermediate coupling approximation.

The present paper employs the diagonalization technique in the intermediate coupling approximation for analyzing the $^1P_1^{(-)}$ and $^3P_1^{(-)}$ self-ionization states of helium-like iron ions, converging to the n = 2 threshold of the residual ion. Together with the electrostatic interaction, in calculating wave functions and excitation energies of the self-ionization states allowance was made for the single-electron part of the spin-orbital interaction which, with increasing Z, rises in proportion to $\alpha^2 Z^4$ (α is the fine structure constant). Inclusion of the spin-orbital interaction results in mixing of singlet and triplet self-ionization states and in the appearance of self-ionization transitions with a change in the total ion spring S which, in the LS coupling approximation are forbidden by the $\Delta S = 0$ selection rule. Here each of the self-ionization levels breaks up into a singlet and triplet states of the continuous spectrum.

The computational scheme used here is as follows. Wave function μ of the self-ionization level, corresponding to a certain value of the total moment J of the system and of its projection M, is represented in the form of a linear combination of suitably symmetrized products of Coulomb functions

$$\Phi_\mu(JM) = \sum_{\gamma_k L_k S_k} C_\mu(\gamma_k L_k S_k)\,\Phi(\gamma_k L_k S_k JM), \qquad (1)$$

the coefficients of which are found by solving the set of algebraic equations

$$\sum_{\gamma_k L_k S_k} \{\langle \gamma_m L_m S_m JM | E_k^0 + \hat{V} - E | \gamma_k Z_k S_k JM\rangle \delta_{L_m L_k}\delta_{S_m S_k} + \langle \gamma_m L_m S_m JM | \hat{H}_{SO} | \gamma_k L_k S_k JM\rangle\} C(\gamma_k L_k S_k) = 0, \qquad (2)$$

where γ is the electron configuration, L is the total orbital moment of the system, V is the operator of interelectron electrostatic interaction, $\hat{H}_{SO}$ is the spin-orbital interaction. In accordance of the diagonalization technique of Balashov et al. [1], the sum in Eq. (2) is restricted to a finite number of terms. The matrix elements of spin-orbital interaction are taken from the book by Yutsis and Savukinas [3], the radial integrals are calculated analytically.

The partial self-ionization widths for transitions to the state of continuous spectrum of different multiplicity are given by the expression

$$\Gamma_{\mu S} = 2\pi |\langle \Phi_{E,S}(r_1, r_2) | \hat{V} | \Phi_\mu(r_1, r_2)\rangle|^2, \qquad (3)$$

where $\Gamma_{\mu,S=0} \equiv \Gamma_0$ corresponds to breakup into singlet, and $\Gamma_{\mu,S=1} \equiv \Gamma_1$ into triplet states of the continuous spectrum; $\Phi_{E,S}(r_1, r_2)$ is the wave function of the continuous spectrum. The sum of partial widths Γ_0 and Γ_1 defines the total width of the self ionization disintegration Γ_{tot}. The spin-orbital relationship between the states of the continuous spectrum with different multiplicity was not incorporated in the calculation.

The algorithm for calculating the matrix elements of operator $\hat{V}$, defining the self-ionization widths and expressed in terms of radial integrals $R(n_1 l_1 n_2 l_2; n_3 l_3 k l_4)$, is based on a scheme of recurrent evaluation of integrals, suggested by Zemtsov [4]. With small modifications this algorithm was also used for evaluating radial integrals $R(n_1 l_1 n_2 l_2; n_3 l_3 n_4 l_4)$ with four functions of the discrete spectrum.

The numerical calculations listed in the table were performed in three versions. In the first of them the wave functions and energies of self-ionization levels were obtained by solving Eqs. (2) with allowance for operators of electrostatic and spin-orbital interaction on a 23 × 23 Coulomb basis, including the $^1P_1^{(-)}$, $^3P_1^{(-)}$ and $^3D_1^{(-)}$ levels of the ten lower configurations $2lnl'$ ($l = 0,1$; $l' = 1,2$; $n \leqslant 5$). In the second version only the electrostatic interaction operator was considered, which corresponds to the LS-coupling approximation, which makes it possible to treat the $^1P^{(-)}$, $^3P^{(-)}$ and $^3D^{(-)}$ states separately. When Eqs. (2) were solved in this approximation a 10 × 10 basis was used for $^1P^{(-)}$ and $^3P^{(-)}$ self-ionization states. In the third version, as in the first allowance was made for the electrostatic and spin-orbital interactions, but only between configurations degenerate in the Coulomb approximation. In all the versions of calculations the width of self-ionization states were calculated with the Coulomb function of the continuous spectrum in the field of charge (Z - 1).

It is seen from the table that incorporation of configuration mixing with respect to the principal quantum number results in insignificant changes in the

Excitation Energies E (keV) and Widths Γ (eV) of Self-Ionization $^1P_1^{(-)}$ and $^3P_1^{(-)}$ States of Helium-Like Fe^{24+} Ions

Terms	Self-ionization states	Present calculations									Perturbation theory [5]
		LS-coupling		Intermediate coupling							
		10×10		23×23					Only degenerate states are included		
		E	Γ	E	Γ_0	Γ_s	Γ_{tot}	$\frac{\Gamma_s}{\Gamma_{tot}}$, %	E	Γ_{tot}	Γ_{tot}
$1p_1^{(-)}$	2s2p	13,629	0,125	13,641	0,121	$0,417\cdot10^{-3}$	0,121	0,34	13,643	0,127	0,129
	23sp—	14,832	$0,228\cdot10^{-3}$	14,826	$0,497\cdot10^{-3}$	$0,776\cdot10^{-3}$	$0,127\cdot10^{-2}$	61,10	14,826	$0,123\cdot10^{-2}$	$0,112\cdot10^{-2}$
	23sp+	14,860	$0,600\cdot10^{-1}$	14,862	$0,565\cdot10^{-1}$	$0,154\cdot10^{-3}$	$0,567\cdot10^{-1}$	0,27	14,863	$0,571\cdot10^{-1}$	$0,581\cdot10^{-1}$
	23d	14,871	$0,313\cdot10^{-3}$	14,874	$0,149\cdot10^{-2}$	$0,764\cdot10^{-4}$	$0,157\cdot10^{-2}$	4,87	14,875	$0,281\cdot10^{-2}$	—
	24sp—	15,262	$0,160\cdot10^{-3}$	15,268	$0,254\cdot10^{-2}$	$0,193\cdot10^{-3}$	$0,273\cdot10^{-2}$	7,07	15,269	$0,274\cdot10^{-2}$	—
	24sp+	15,273	$0,263\cdot10^{-1}$	15,277	$0,212\cdot10^{-1}$	$0,953\cdot10^{-4}$	$0,213\cdot10^{-1}$	0,45	15,277	$0,192\cdot10^{-1}$	—
$3p_1^{(-)}$	2s2p	13,599	$0,944\cdot10^{-2}$	13,590	$0,481\cdot10^{-2}$	$0,116\cdot10^{-1}$	$0,164\cdot10^{-1}$	29,33	13,591	$0,168\cdot10^{-1}$	$0,134\cdot10^{-1}$
	23sp+	14,840	$0,494\cdot10^{-2}$	14,836	$0,407\cdot10^{-2}$	$0,335\cdot10^{-2}$	$0,742\cdot10^{-2}$	54,85	14,837	$0,757\cdot10^{-2}$	—
	23sp—	14,841	$0,149\cdot10^{-3}$	14,839	$0,616\cdot10^{-3}$	$0,193\cdot10^{-2}$	$0,255\cdot10^{-2}$	24,16	14,839	$0,249\cdot10^{-2}$	—
	23d	14,862	$0,251\cdot10^{-7}$	14,866	$0,404\cdot10^{-3}$	$0,401\cdot10^{-5}$	$0,408\cdot10^{-3}$	99,02	14,867	$0,427\cdot10^{-3}$	—
	24sp+	15,265	$0,209\cdot10^{-2}$	15,252	$0,130\cdot10^{-2}$	$0,560\cdot10^{-3}$	$0,186\cdot10^{-2}$	69,89	15,252	$0,171\cdot10^{-2}$	—
	24sp—	15,267	$0,133\cdot10^{-3}$	15,264	$0,207\cdot10^{-2}$	$0,153\cdot10^{-2}$	$0,360\cdot10^{-2}$	57,50	15,264	$0,349\cdot10^{-2}$	—

excitation energies and widths of the self-ionization levels under study, whereas inclusion of the spin-orbital interaction affects their characteristics significantly. The ratio of partial widths, corresponding to self ionization transitions with change in multiplicity, to the total widths of the self-ionization levels shows that the widths of triplet self-ionization states change more in this case. It is seen by comparing the present results with calculations performed on the basis of the perturbation theory, and including completely the Breit operator [5], that when the widths of self-ionization levels of iron are calculated in the intermediate-coupling approximation, it is possible to retain solely the single-particle operator of spin-orbital interaction.

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