Relativistic calculation for photoionization of the ground state of neonlike Fe XVII

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Relativistic calculations are made for photoionization of the ground state of neonlike Fe XVII, using the Breit-Pauli Hamiltonian within the R-matrix method. Relativistic effects are clearly revealed by comparing the results with those obtained in the nonrelativistic LS coupling approximation. [S1050-2947(98)08204-3]

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I. INTRODUCTION

The interaction of electrons and photons with ionized atoms, particularly with metallic impurities such as Ti, Cr, Fe, and Ni, plays an important role in controlled thermonuclear plasmas, as discussed recently [1]. The study of neonlike iron Fe XVII has also attracted considerable interest in astrophysics, since strong emission lines from this ion have been observed in the solar corona and in solar flares [2].

In the present work, we have made a relativistic calculation of the photoionization cross section from the ground state $1s^2 2s^2 2p^6\ {}^1S_0^e$ of Fe XVII, by using the close-coupling Breit-Pauli R-matrix method [3]. In the R-matrix formulation of photoionization [4], the initial bound state of Fe XVII and the final continuum states consisting of the residual ion Fe XVIII plus an outgoing electron are expanded consistently on collision-type R-matrix basis sets, expressed in terms of the states of the N-electron residual ion Fe XVIII. The three lowest states $1s^2 2s^2 2p^5\ {}^2P_{3/2}^o$, $1s^2 2s^2 2p^5\ {}^2P_{1/2}^o$, $1s^2 2s 2p^6\ {}^2S_{1/2}^e$ have been included in the expansion of the initial and final states, allowing for the following direct phoionization processes:

$$\text{Fe XVII}(2s^2 2p^6 1S^e,\ J=0^e)+h\nu$$

$$\rightarrow|\text{Fe XVIII}(2s^2 2p^6\ {}^2P_{3/2}^o)+e(s,d)|,\quad J=1^o, \tag{1a}$$

$$\rightarrow|\text{Fe XVIII}(2s^2 2p^5\ {}^2P_{1/2}^o)+e(s,d)|,\quad J=1^o, \tag{1b}$$

$$\rightarrow|\text{Fe XVIII}(2s 2p^6\ {}^2S_{1/2}^e)+e(p)|,\quad J=1^o, \tag{1c}$$

as well as the formation of the following Rydberg series:

$$\rightarrow|\text{Fe XVIII}^*(2s^2 2p^5\ {}^2P_{1/2}^o)n(s,d)|,\quad J=1^o, \tag{2a}$$

$$\rightarrow|\text{Fe XVIII}^{**}(2s 2p^6\ {}^2S_{1/2}^e)np|,\quad J=1^o \tag{2b}$$

below the two excited ionization thresholds. As shown later on, the formation of strong Rydberg series of autoionized resonances (2a) below the excited fine structure level of the ground configuration $2s^2 2p^5\ {}^2P_{1/2}^o$ is a pure relativistic effect that modifies considerably the photoionization cross section below 1 Ry for the energy of the ionized electron.

II. DETAILS OF THE CALCULATION

The fluorinelike target state $2s^2 2p^5\ {}^2P_{3/2,1/2}^o$ and $2p^6\ {}^2s_{1/2}$ residual ion Fe XVIII have been represented by intermediate coupling LSJ configuration expansions [5],

$$\Phi(J)=\sum_{i=1}^{M} a_i \phi_i(\alpha_i, LSJ), \tag{3}$$

where the single configuration functions ϕ_1 are constructed from one-electron orbitals, whose angular momenta are coupled as specified by α_1 to form states of given total L, S, and J. The radial part of each orbital is written as a linear combination of normalized Slater-type orbitals (STO):

$$P_{nl}=\sum_{i=i}^{k} b_i \left[\frac{(2\zeta_i)^{2p_i+1}}{(2p_i)!}\right]^{1/2} r^{p_i}\exp(-\zeta_i r), \tag{4}$$

which satisfy the following orthonormality conditions:

$$\int_0^\infty P_{nl}P_{n'1'}dr=\delta_{nn'}\delta_{ll}. \tag{5}$$

In the present calculation, we have used a restricted basis of 3 STO, $1s$, $2s$, $2p$ optimized on the ground state of the Fe XVIII fluorine-like ion by Clementi and Roetti [6] and single LSJ representations of the three Fe XVIII states included in the calculation [Eq. (1)]. The energies of the corresponding states in the Breit-Pauli approximation are defined by

$$\langle\Phi_i(J)|H_{\text{BP}}^N|\Phi_i(J')\rangle=E_i^N\delta_{JJ}, \tag{6}$$

where we include the mass correction, monoelectronic Darwin and spin-orbit terms of the Breit-Pauli approximation:

$$H_{\text{BP}}^N=H_{\text{NR}}^N+H_{\text{mass}}^N+H_{D_1}^N+H_{\text{SO}}^N \tag{7}$$

TABLE I. Energies (Ry) of fine-structure level of $2p^5$. $2s2p^6$ in Fe XVIII.

Key	Configuration	Theoretical	Experimental
1	$2p^5\ ^2P^o_{3/2}$	0.00000	0.00000
2	$2p^5\ ^2P^o_{1/2}$	1.03026	0.9354
3	$2s2p^6\ ^2S^o_{1/2}$	9.85300	9.7013

with

$$+H^N_{\rm mass}=-\frac{1}{8}\,\alpha^2\sum_{i=1}^{N}\nabla_i^4, \tag{8a}$$

$$+H^N_{D_1}=-\frac{1}{8}\,\alpha^2 Z\sum_{i=1}^{N}\nabla_i^2\left(\frac{1}{r_i}\right), \tag{8b}$$

$$+H^N_{\rm SO}=+\frac{1}{2}\,\alpha^2 Z\sum_{i=1}^{N}\vec{1}_i\,\frac{\vec{s}_i}{r_i^3}. \tag{8c}$$

These Breit-Pauli energies are compared in Table I with their LS counterparts and with the experimental values tabulated by Wiese [7]. It can be seen in Table I that the LSJ excitation energies are in fair agreement with experiment.

The differential cross section for photoionization of an $(N+1)$-electron atom with the electron ejected in direction $\vec{k}$ and the ion left in state f is given by [3]

$$\frac{d\sigma_f}{d\vec{k}}=8\pi^2\alpha a_0^2\omega\left|\left\langle\psi_f^-(\vec{k})\left|\sum_{i=1}^{N+1}\vec{r}_i\psi_i\right\rangle\right|, \tag{9}$$

where ω is the photon energy in a.u., α is the fine-structure constant, a_0 is the Bohr radius, ψ_i is the wave function of the initial bound state, and $\psi_f^-(\vec{k})$ is the wave function of the final state with a single outgoing wave corresponding to the ejected electron in direction $\vec{k}$ and the residual ion in state f.

As described by Burke and Taylor [3], in the R-matrix theory of photoionization, both the initial bound state ψ_i and the final continuum state $\psi_f(\vec{k})$ are expanded in terms of discrete R-matrix basis sets.

TABLE II. Configurations used in CI expansion of Fe XVIII target states.

Target states	Key no.	Configuration used
$^2P^o$	1,2	$[1s^2]2s^22p^5$, $2s^22p^4(^3P)3p$, $2s^22p^4(^1D)3p$, $2p^4(^1S)3p$, $2p^5(^2P^o)3s^2$, $2p^5(^2P^o)3p^2$
$^2S^e$	3	$2s2p^6$, $2s2p^5(^3P^o)$, $2s2p^5(^1P^o)3p$, $2s^22p^4(^1S)3s$, $2s^22p^4(^1D)3d$, $2p^6(^1S)3s$

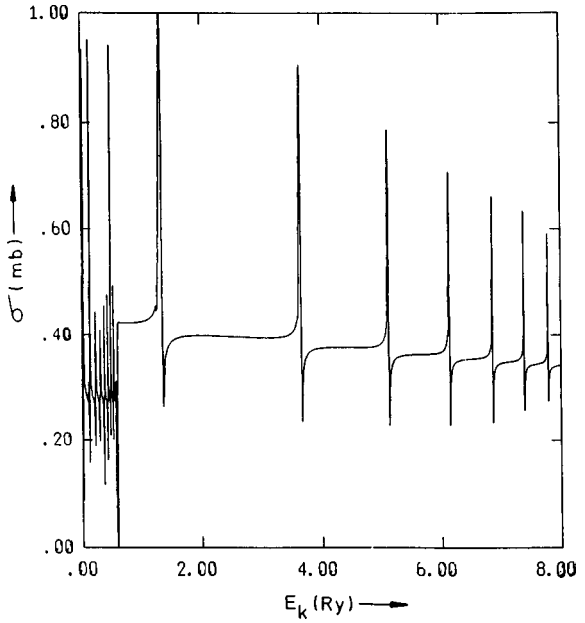

FIG. 1. Photoionization cross section in Mb for the photoionization from the ground state of Fe XVII in the relativistic LSJ coupling as a function of the photoelectron energy E_k (in Ry) in the energy region from $2s^22p^5\ ^2P^o_{3/2}$ threshold to near $2s2p^6\ ^2S_{1/2}$ threshold of Fe XVII.

$$\psi_k=\mathcal{A}\sum_{ij}\,c_{ijk}\Phi_i(X_1\cdots X_N,\hat{r}_{N+1},\sigma_{N+1})u_{ij}{}^{(r_{N+1})}$$

$$+\sum_j\,d_{jk}\phi_j(X_1\cdots X_{N+1}), \tag{10}$$

inside a sphere of radius a containing the charge distribution of the residual ion. In Eq. (10), $\mathcal{A}$ is the antisymmetrization operator that accounts for electron exchange. Φ_i are channel functions formed by coupling the target states (see Table II)

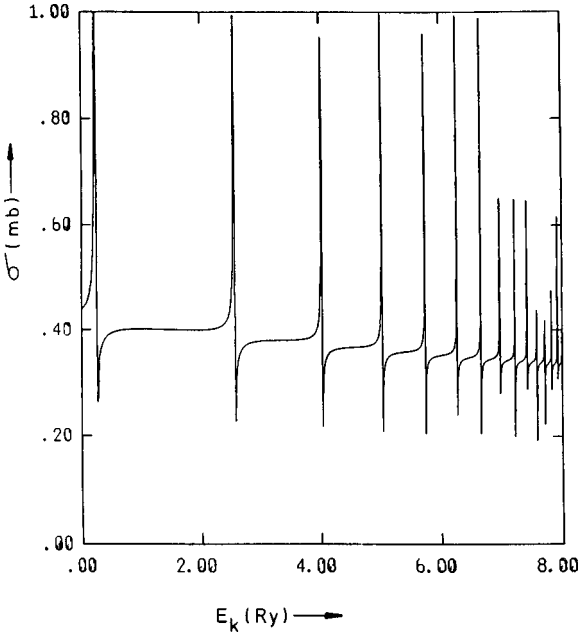

FIG. 2. Same as for Fig. 1, but the resolved pattern for E_k from 0.50 Ry is shown.

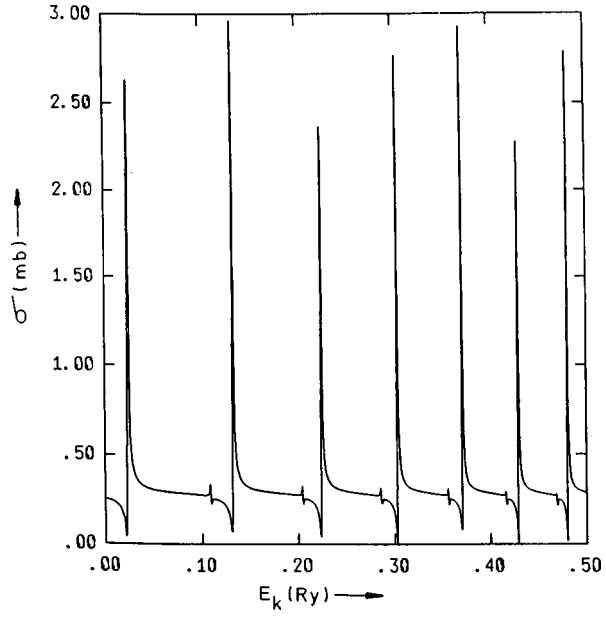

FIG. 3. Same as for Fig. 1, but in the nonrelativistic-LS coupling.

of coordinates $x_i=\{r_i,\hat{r}_i,\sigma_i\}$ with the spin angle function of the scattered electron in order to form eigenstates of the total angular momentus J_t and parity π_t. More precisely, following Burke and Scot [3] the pair coupling scheme

$$\vec{J}+\vec{l}=\vec{K}, \quad \vec{K}+1/2=\vec{J}_t \tag{11}$$

is used, since this coupling scheme is expected to be approximately realized in medium size atomic systems. The $\{u_{ij}\}$ form a discrete R-matrix basis of continuum orbitals for the scattered electron and the $\{\Phi_j\}$ are $(N+1)$-electron bound configurations, which account for the orthogonality of the continuum orbitals u_{ij} to the bound orbitals.

The continuum orbitals u_{ij} in Eq. (10) are eigenfunctions of a zero-order, nonrelativistic model Hamiltonian:

$$\left[-\frac{d^2}{dr^2}+\frac{1_i(l_i+1)}{r^2}+2V(r)-k_i^2\right]u_{ij}(r)=\sum_k \lambda_{ijk}p_k(r), \tag{12a}$$

which satisfy the following boundary conditions:

$$u_{ij}(0)=0, \tag{12b}$$

$$\frac{a}{u_{ij}}\frac{du_{ij}}{dr}\bigg|_{r=a}=b. \tag{12c}$$

In Eq. (12a) l_i is the angular momentum of the scattered electron, $V(r)$ is the static potential of the target in its ground state, and λ_{ijk} are Lagrange multipliers, which are determined in order to ensure the orthogonality of the continuum orbitals to the bound radial orbitals $P_{kl},(r)$ having the same angular momentum l_i. We imposed a zero logarithmic derivative $b=0$ at the R-matrix boundary radius $a=3.4$ a.u. and we retained 15 continuum orbitals for each angular symmetry, to ensure convergence in the energy range considered here, namely, up to 25 Ry.

TABLE III. Cross section from the ground state for ejected electron kinetic energy from 10 to 24 Ry in LS coupling and LSJ coupling. Ion threshold in LS coupling is -92.73 Ry while in LSJ coupling it is -93.55 Ry.

Energy (Ry)	Nonrelativistic LS coupling	Relativistic intermediate LSJ coupling
10.0	0.38234	0.37311
12.0	0.36444	0.35553
14.0	0.34775	0.33992
16.0	0.33242	0.32640
18.0	0.31829	0.31437
20.0	0.30505	0.30285
22.0	0.29238	0.29100
24.0	0.26833	0.27859

The coefficients c_{ijk} and d_{jk} in Eq. (9) were determined by diagonalizing the $(N+1)$-electron Breit-Pauli Hamiltonian matrix [Eqs. (5) and (6) for $N+1$ electrons] in the inner region. In the outer region $(r\geqslant a)$, the radial equations were solved, assuming a purely Coulombic asymptotic interaction.

III. RESULTS AND DISCUSSION

The present results have been obtained, using a fine mesh of 0.01 in effective quantum number:

$$n_{\text{eff}}=\sqrt{2(E-E_f)}/\mathcal{Z} \tag{13}$$

for kinetic energies E of the ejected electron smaller than energy E_f of an excited state f of the residual ion, in order to resolve the series of autoionizing resonances converging to their corresponding thresholds, while, above all the included thresholds, a coarse mesh in energy E was used.

Figure 1 shows the total photoionization cross section in Mb as a function of the kinetic energy of the ejected electron in Rydbergs in the energy range from the first ionization threshold $^2P^o_{3/2}$ to 8 Ry, below the third threshold $^2S_{1/2}$ and Fig. 2 shows the same cross section on an expanded energy scale below the excited fine-structure threshold $^2P^o_{1/2}$. As expected, the cross section is strongly affected by a series of unperturbed autoionized Rydberg resonances [8]. Below the first excited fine-structure threshold $^2P^o_{1/2}$ that occurs around 1 Ry, about one-third of the oscillator strength density is concentrated into a strong series of $^2P^o_{1/2}nd_{3/2}$ resonances and weaker series of $^2P^o_{1/2}ns_{1/2}$ resonances on the left side of the resonances, as suggested by the effective quantum numbers 16.94 and 17.70 of the first two resonances. It is found that the d resonances are considerably broader than the s resonances.

The resonances occurring below the third threshold $2s2p^6\ ^2S^e_{1/2}$ correspond to the temporary capture of a p electron, as suggested by the effective quantum number of the first resonance being 5.81. Their dispersion shape is very similar to that obtained in the nonrelativistic LS approximation, given in Fig. 3. We note that above the $^2P^o_{1/2}$ state, practically the only difference between the relativistic (Fig. 1) and nonrelativistic (Fig. 3) results arises from the shift of

the third threshold, which is expected due to the inclusion of relativistic one-body operators.

Above the third excitation thresholds, the cross sections decrease slowly. Table III compares the partial cross sections for leaving the residual ion in one of its allowed final states in the nonrelativistic and relativistic approximations. Both the results agree with each other within 3%.

In conclusion, in this calculation on photoionization of Fe XVII from the ground state, all the important physical effects such as exchange, channel coupling, short range correlations, and relativistic effects [9] have been included.

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