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Theoretical study on the K_α transition properties of F-like ions

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Abstract. In a recent calculation on K_α transition properties of fluorine-like ions ($10 \leq Z \leq 79$) by Sur *et al*. [Phys. Rev. A 77 (2008) 052502], it was found that there is a crossover between $K_{\alpha 1}$ and $K_{\alpha 2}$ transition probabilities with increasing of atomic number Z. In order to examine this unusual behavior, a further theoretical study has been carried out by using multi-configuration Dirac-Fock (MCDF) method. In the calculation, Breit interaction, electron correlation and quantum electrodynamics (QED) effects have been included. The present study shows a contrary conclusion to the earlier theoretical results.

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Key words: F-like ions, K_α transition, Breit interaction, QED effect, MCDF method

1 Introduction

X-ray emission is a phenomenon resulting from the decay of atoms after bombardment by charged particles or electromagnetic radiation. The study of this phenomenon is very important for many fields. For example, the K-shell X-ray provides new ways in diagnostics on temperature, density, opacity, and charge distributions in plasmas [1]. Meanwhile, an accurate measurement of the relative intensities for K_α X-rays is of importance to test the relevant existing theories [2]. Furthermore, a precise determination of X-ray energies for transitions into ground state of a high-Z hydrogen-like ion is the most direct experimental approach for the investigation of the quantum electrodynamics (QED) effects in strong Coulomb field [3]. Of course, their importance in biomedical research as well as in X-ray astronomy is also pointed out [4–7]. F-like ions can give rise to K_α transition when there is a vacancy in K shell. Many studies have been done for F-like ions in both experimental observations and theoretical calculations [1, 8–19], but most of these works

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focused on spin-orbit intervals in the ground states. Therefore, it is necessary to perform a comprehensive theoretical research on F-like ions, including the ground-state fine structures, K_α transition energies and probabilities.

From a theoretical point of view, precise wavefunctions must be used for both the initial states and the final states to obtain accurate transition probabilities, but for a highly charged heavy ion with few electrons, relativistic and electron correlation effects must be treated, which poses a considerable challenge for obtaining an exact wavefunction [9]. So, in order to get more reliable information about the transition processes, large wavefunction expansions are often needed [20]. In ab initio calculations, these wavefunctions must include the most dominant physical effects, such as relativity, electron correlations, and relaxation within a common framework [21].

In this paper, we have calculated the doublet splitting of $1s^2 2s^2 2p^5\ ^2P_{3/2,1/2}$, and determined the contributions of both Breit interaction and QED effects to the transition energies from $1s2s^2 2p^6\ ^2S_{1/2}$ to $1s^2 2s^2 2p^5\ ^2P_{3/2,1/2}$ for F-like ions ($16 \leq Z \leq 92$). Much attention has been paid to the K_α transition probabilities. The fully relativistic multi-configuration Dirac-Fock (MCDF) method [22, 23] has been used to calculate exact wavefunctions, and the recently developed REOS99 program [24] has been used to compute transition energies and probabilities. The structure of this paper is as follows. In Section 2, we briefly introduce the method applied in the present calculations. The calculated results and discussion are given in Section 3. Also the conclusion is given in Section 4.

2 Theoretical method

In this study, wavefunctions have been generated by using the widely used relativistic atomic structure package GRASP92 [25], on the basis of the MCDF method in which an atomic state is approximated by a linear combination of configuration state functions (CSFs) with the same symmetry

$$|\Psi_\alpha(PJM)\rangle = \sum_{r=1}^{n_c} c_r(\alpha)|\gamma_\alpha(PJM)\rangle, \tag{1}$$

where n_c is the number of CSFs and $c_r(\alpha)$ denotes the representation of the atomic state in this basis. In a standard calculation, the CSFs are the antisymmetrized products of a common set of orthonormal orbitals which are optimized on the basis of the Dirac-Coulomb Hamiltonian. Further relativistic contributions to the representation $c_r(\alpha)$ of the atomic states due to (transverse) Breit interactions are added by diagonalizing the Dirac-Coulomb-Breit Hamiltonian matrix. And the dominant QED contributions to the transition energies have been included as a perturbation.

The Einstein spontaneous emission probability for transition from initial state β to final state α can be given by

$$A_{\alpha\beta} = \frac{2\pi}{2J_\beta + 1} \sum_{M_\alpha} \sum_{M_\beta} |M^{(L)}_{\alpha\beta}|^2, \tag{2}$$