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Electric dipole transitions for highly excited states in helium-like sulphur

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Abstract

We have calculated relativistic energies, weighted oscillator strengths and transition probabilities for electric dipole (E1) transitions among the terms belonging to $1snl$ ($n \leqslant 9$, $l \leqslant 3$) configurations in helium-like sulphur. The calculations are based upon the multiconfiguration Hartree–Fock method within the framework of Breit–Pauli relativistic corrections. Our calculated values are also compared with other experimental and theoretical results.

Keywords: MCHF method; Relativistic correction; Transition energies; Wavelengths; Oscillator strengths; Transition probabilities

1. Introduction

Oscillator strengths (*f*-values) and transition probabilities or lifetime subjects have been frequently studied. These subjects are especially important for astrophysics. For instance, oscillator strengths are needed to convert amount of absorption into abundances in fields ranging from fusion to interstellar and stellar astrophysics. We learn about the species' electronic structure from these data. Data about these subjects including theoretical computations, laboratory experiments and astronomical measurements for most atoms were compiled (see, for example, [1–4]).

Some excited states of two-electron atoms have been widely studied in the literature. There are a lot of studies for lower states of helium-like sulphur (S XV, $Z = 16$). Oscillator strength values of 1^1S, 2^1P and 2^3S, and 2^3P transitions were obtained by Sanders and Scherr [5]. The helium-like sulphur in the solar spectrum was observed by Walker and Rugge [6]. Drake [7] calculated relativistic magnetic dipole transitions for the 2^3S state. Brown and Cortez [8] obtained oscillator strengths for allowed nd–$n'f$ transitions in the helium-like isoelectronic sequence. Lifetimes of the 2^3P_2 and 2^3S_1 states by X-ray emission were measured by Cocke et al. [9] and Bednar et al. [10]. Allowed and forbidden radiative transitions were studied with a relativistic version of the random-phase approximation by Johnson and Lin [11]. Varghese et al. [12] reported measurements of the lifetime of the 2^3P_1 state using the trace-of-flight technique. The strengths of various decay modes and energy splittings of $n = 2$ multiplets were investigated with RRPA by Lin et al. [13]. Boiko et al. [14] observed

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the wavelengths and relative intensities of the intercombination lines $3^3P_1 \rightarrow 1^1S_0$ in the spectra of laser-produced plasma. Lin et al. [15] calculated oscillator strengths for the transitions $m^{3,1}S_{0,1}$–$n^{3,1}P_1$ ($3 \leqslant m$, $n \leqslant 5$). Mewe and Schrijver [16] evaluated line intensities of all lines for helium-like ions. Drake [17] presented frequencies and transition rates in some helium-like ions. Berry et al. [18] analyzed wavelengths and fine structure of $2s$–$2p$ transition in two-electron ions and compared them with theory and experiments. The wavelengths of 2^3S–2^3P transitions in S XV were measured by Livingston et al. [19]. Precision wavelength measurements for 2^3S_1–$2^3P_{0,2}$ transitions and 2^1P_1–1^1S_0 and 2^3P_1–1^1S_0 transition in helium-like sulphur were presented by DeSerio et al. [20] and Schleinkofer et al. [21]. Energy levels for $1snl$ ($n = 2$–5) states were calculated the perturbation method by power series in $1/Z$ and αZ by Vainshtein and Safronova [22]. A theoretical study of two-photon emission rates for the 2^1S state and $n = 1$ and 2 states were presented by Drake [23,24]. A comparison between calculated and measured wavelengths of resonance transitions were reported by Aglitsky et al. [25]. The energies of the $n = 2$ triplet states in helium-like ions were calculated with relativistic many-body perturbation theory by Johnson and Sapirstein [26]. Berry et al. [27] made a careful comparison of the triplet state energies. The results for relativistic configuration–interaction calculations of $n = 2$ triplet states of helium-like ions were presented by Chen et al. [28]. Relativistic many-body calculations of $n = 1$ and 2 states were observed by Plante et al. [29]. The list of wavelengths, oscillator strengths and statistical weights for spectral lines arising from the ground state were presented by Verner et al. [30]. Howie et al. [31] measured the wavelengths using photographic spectroscopy of beam foil $n = 2$ triplet states. Kato et al. [32] reported theoretical atomic data of satellite spectra for helium-like sulphur with different methods. Two-photon decay rates of metastable 2^1S_0 and 2^3S_1 states were presented for helium-like ions in the $Z = 2$–100 range by Derevianko and Johnson [33]. Safronova and Johnson [34] studied energy levels and autoionizing rates of some levels for helium-like with $Z = 4$–54 ions. Kimura et al. [35] calculated rate coefficients for electron impulse excitation of helium-like ions with the Dirac R-matrix approach. Kingston et al. [36] obtained spontaneous transition rates for E1, M1, E2 and M2 transitions using fully relativistic GRASP and CIV3 codes.

In the theoretical study of atomic structure, there are two interesting subjects: one deals with the electron correlation and the other deals with the relativistic effects. In this work, we are interested in both subjects mentioned above. The work is organized as follows. It is used the multiconfiguration Hartree–Fock (MCHF) approximation within the framework of Breit–Pauli relativistic corrections in helium-like sulphur. We selected $1sns$ ($1 \leqslant n \leqslant 9$) and $1snd$ ($3 \leqslant n \leqslant 9$) for even-parity states, and $1snp$ ($2 \leqslant n \leqslant 9$) and $1snf$ ($4 \leqslant n \leqslant 9$) for odd-parity states to consider core–valence correlation effects. We obtained the 1526 possible E1 transitions. In other words, we report a large-scale calculation for highly excited and ionized sulphur (S XV). The results obtained for lower states are compared with other available data and new results for highly excited states are also presented.

2. Calculation method

The MCHF approximation is a configuration–interaction method given by Fischer [37]. In this approximation the MCHF Hamiltonian is used for obtaining the best radial functions for the set of non-relativistic energies of the interacting terms. Then, the Breit–Pauli wavefunctions are obtained as a linear combination

$$\Psi(\gamma JM_J) = \sum_{i=1}^{M} c_i \Phi(\gamma_i L_i S_i JM_J), \quad \sum_{i=1}^{M} c_i = 1,$$

where $\Phi(\gamma LSJM_J)$ are LSJ-coupled configuration state functions (CSFs), that is

$$\Phi(\gamma LSJM_J) = \sum_{M_L M_S} \langle LM_L SM_S | LSJM_J \rangle \Phi(\gamma LM_L SM_S),$$

where γ_i denotes configurations; the orbital L_i and the spin S_i angular momenta are coupled to give the total angular momentum J. The mixing (or expansion) coefficients c_i are obtained by diagonalizing the Breit–Pauli Hamiltonian. The radial functions building the CSFs are taken from previous non-relativistic MCHF