Calculations of the transition energies and oscillator strengths for Cu^{26+} ion

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Abstract. Non-relativistic energies of $1s^2 2s$ and $1s^2 np$ ($n \leq 9$) states for Cu^{26+} ion are calculated by using the full-core plus correlation method. For $1s^2 2s$ and $1s^2 2p$ states, relative discrepancies between our results and high precision results of Yan *et al.* are within 0.1 ppm. By taking account of the first-order corrections to the energy from relativistic and mass-polarization effects, the higher-order relativistic contribution and QED correction to the energy are estimated under a hydrogen-like approximation. The transition energies, wavelengths and oscillator strengths for the $1s^2 2s - 1s^2 np$ transitions of the ion are calculated. The results obtained by the three forms are in good agreement with each other.

1 Introduction

The research on the structures and properties of highly ionized atomic systems is of fundamental importance in atomic physics and plays an important role in other fields such as astrophysics, plasma physics, laser physics and so on. In addition, this subject also provides a challenge to theoretical work because there are significant differences between the features of these systems and of neutral or lowly ionized systems [1, 2]. In recent years, there have been several reports of calculations of energies and oscillator strengths for lithium-like ions [3–6]. Particularly, the high-precision energies and oscillator strengths of $1s^2 2s - 1s^2 2p$ for Li-like systems up to $Z = 50$ were given by Yan *et al.* [3] using the Hylleraas-type variational method and the $1/Z$ expansion method. However, for lithium-like ions with higher Z, particularly for their excited states, there is little information available in literatures.

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In recent years, we calculated the energies and oscillator strengths of some ions and obtained some satisfactory results [7–9]. In this paper, the non-relativistic energies of $1s^2 2s$ and $1s^2 np$ ($n \leq 9$) states for Cu^{26+} ion are calculated by using the full-core plus correlation (FCPC) method [10]. By evaluating the first-order corrections to the energy from the relativistic and mass-polarization effects by using the perturbation theory, the higher-order relativistic contribution and QED correction to the energy are estimated under a hydrogen-like approximation. The transition energies, wavelengths and oscillator strengths of $1s^2 2s - 1s^2 np$ for this ion are calculated. The comparisons of our theoretical results with experimental data available in literatures are carried out.

2   Computation

The details of the FCPC method have been given by Chung [10], which will not be repeated here. The wave functions of $1s^2 nl$ ($l = s$, and p) states for lithium-like Cu^{26+} ion are given by

$$\Psi(1,2,3) = A\left[\Phi_{1s1s}(1,2)\sum_i d_i r_3^i e^{-\beta r_3} Y_{l(i)}(3)\chi(3) + \sum_i C_i \Phi_{n(i),l(i)}(1,2,3)\right], \qquad (1)$$

where A is an antisymmetrization operator. $\Phi_{1s1s}(1,2)$ is the predetermined $1s^2$-core wave function, and its expression can be found in Ref. [10]. The second term on the right hand side of Eq. (1) describes other possible correlations and the relaxation of $1s^2$-core in the system. $\Phi_{n(i),l(i)}$ is the basis set of three electron system. The non-relativistic energies (upper bounds) E_0 of the $1s^2$-core and $1s^2 nl$ states are calculated by minimizing the expectation value of non-relativistic Hamiltonian operator whose explicit expression is given in Ref. [10]. Their corresponding FCPC wave functions Ψ are determined in this process.

The corrections ΔE to energy of these states from relativistic and mass-polarization effects are calculated by using the first-order perturbation theory,

$$\Delta E = \Delta E_1 + \Delta E_2, \qquad (2a)$$

$$\Delta E_1 = <\Psi|H_1 + H_2|\Psi>, \qquad (2b)$$

$$\Delta E_2 = <\Psi|H_3 + H_4 + H_5|\Psi>, \qquad (2c)$$

where ΔE_1 is the first-order corrections from the one-particle operators including the correction to kinetic energy and Darwin term, and ΔE_2 is the contributions from two-particle operators, including the electron-electron contact term, the orbit-orbit interaction and the mass-polarization effect. The expressions of these operators are also given in Ref. [10]. In order to obtain more accurate results for the system with higher Z, QED and higher-order relativistic effects on the energy should be taken account. As is known, the energy eigenvalue of one-electron Dirac equation (excluding the rest mass energy) for a