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Fine structures of $1s^2np$ and $1s^2nd$ states for Zn^{27+} ion

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Abstract. The non-relativistic energies and wavefunctions of $1s^2np$ and $1s^2nd$ states for Zn^{27+} ion are obtained by using the full-core plus correlation method. The expectation values of the spin-orbit and spin-other-orbit interaction operators in these states are calculated. By introducing the effective nuclear charge, the higher-order relativistic contribution and QED correction to the fine structure splittings are estimated.

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Key words: Zn^{27+} ion, fine structure, higher-order relativistic and QED corrections

1 Introduction

The structures and properties of highly ionized atomic systems have many characteristics different from that of neutral or lowly ionized atoms [1]. One among them is the fine structure splitting which rapidly grows to become "not-so-fine" [2]. As knows, the basic physical mechanism leading to fine structure is the spin-orbit interaction, the scaling of which is proportional to four powers of effective nuclear charge isoelectronically.

In this paper, by using the wavefunctions determined in calculating non-relativistic energies of $1s^2np$ and $1s^2nd$ states for Zn^{27+} ion with the full-core plus correlation (FCPC) method [3], the expectation values of the spin-orbit and spin-other-orbit interaction operators, as the first-order approximation of fine structure splitting in $1s^2np$ and $1s^2nd$ states for Zn^{27+} ion, are calculated. The higher-order relativistic contribution and QED correction to the fine structure splittings are estimated by introducing the effective nuclear charge. The contributions to the fine structure splittings from the first-order approximation, the higher-order relativistic, and QED correction, which given respectively in a table, are quantitatively analyzed.

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2 Theoretical method

The wavefunctions of $1s^2np$ and $1s^2nd$ states for lithiumlike Zn^{27+} ion are given by [3]

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

The details of every terms in Eq. (1) can be found in Ref. [3]. The parameters in Eq. (1) are determined by solving the secular equation of the system. In this process, the FCPC-type wavefunctios, Eq. (1) , of $1s^2np$ and $1s^2nd$ states for Zn^{27+} ion are completely determined.

The first-order approximation of fine structure splitting in $1s^2np$ and $1s^2nd$ states for the ion is given by the expectation values of the spin-orbit and spin-other-orbit interaction operators which are

$$H_{\mathrm{SO}}=\frac{Z}{2c^2}\sum_{i=1}^{3}\frac{\mathbf{l_i}\cdot\mathbf{s_i}}{\mathbf{r}_i^3}, \tag{2}$$

$$H_{\mathrm{SOO}}=-\frac{1}{2c^2}\sum_{i\neq j}^{3}\left[\frac{1}{r_{ij}^3}\left(\mathbf{r}_i-\mathbf{r}_j\right)\times\mathbf{p}_i\right]\cdot\left(\mathbf{s}_i+2\mathbf{s}_j\right). \tag{3}$$

The effective nuclear charge, Z_{eff}, affected by nl $(l=p$, and $d)$ electron in the system can defined as follows [4–7]

$$\begin{aligned}&E_{\mathrm{non-rel1}}(1s^2nl)+\Delta E_1(1s^2nl)-E_{\mathrm{non-rel}}(1s^2)-\Delta E_1(1s^2)\\&=-\frac{Z_{\mathrm{eff}}^2}{2n^2}\left[1+\frac{\alpha^2 Z_{\mathrm{eff}}^2}{n}\left(\frac{1}{k}-\frac{3}{4n}\right)\right],\end{aligned} \tag{4}$$

where ΔE_1 is the contributions from the expectation values of one-particle operators including the correction to kinetic energy and Darwin term. The explicit expressions of these two operators can be found in Refs. [3, 8]. The higher-order relativistic contribution to the fine structure splittings are estimated in terms of the following equation

$$\Delta E_{\mathrm{higher-order}}=E_{\mathrm{Dirac}}(Z_{\mathrm{eff}})-E^{(1)}(Z_{\mathrm{eff}}), \tag{5}$$

where E_{Dirac} is the eigenvalue of one-electron Dirac equation in Coulomb potential [8] which can be reduced to $E^{(1)}$ if the $\alpha^2 Z^4$-order contribution is only retained.

By using Z_{eff} defined in Eq. (4), QED correction to the fine structure splittings can be also evaluated [8]

$$\Delta E_{\mathrm{QED}}^{\mathrm{FS}}=\frac{\alpha^3 Z_{\mathrm{eff}}^4}{2\pi n^3}\cdot\frac{C_{lj}}{(2l+1)}, \tag{6}$$

where

$$C_{lj}=\frac{\delta_{j,l+\frac{1}{2}}}{l+1}-\frac{\delta_{j,l-\frac{1}{2}}}{l}. \tag{7}$$