J. At. Mol. Sci.
doi: 10.4208/jams.032211.041611a

Vol. **3**, No. 1, pp. 59-63
February 2012

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

Zhi-Wen Wang*, Yuan-Yuan Qi, and Lei Sha

School of Physics and Electronic Technology, Liaoning Normal University, Dalian 116029, China

Received 22 March 2011; Accepted (in revised version) 16 April 2011
Published Online 28 September 2011

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.

PACS: 32.10.Fn, 31.25.Jf, 31.70.Cs

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.

*Corresponding author. *Email address:* zh.w.wang@163.com (Z. W. Wang)

2 Theoretical method

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

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

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

$$H_{\rm SO}=\frac{Z}{2c^2}\sum_{i=1}^{3}\frac{\mathbf{l_i}\cdot\mathbf{s_i}}{\mathbf{r}_i^3}, \quad (2)$$

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

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

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

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

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

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

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

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

where

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

3 Results and discussion

We used 222 terms in seven l components for the $1s^2$-core wave function, and ten and nine d_i terms in Eq. (1) for $1s^2np$ and $1s^2nd$ states respectively. The number of terms in $\Phi_{n(i),l(i)}$ ranges from 979 to 854 in 17 partial waves for these states.

Our calculated results of fine structure splittings for $1s^2np$ and $1s^2nd$ states of Zn^{27+} ion are listed in Table 1. For $1s^22p$ state, our result, 238686.51 cm^{-1}, agrees closely with the experimental datum, 239086 cm^{-1} [9]. We have reason to believe that our theoretical predictions of the splittings for other states should be accurate enough, although there are not experimental data in the literature for these cases yet. It is hoped that these predictions may provide a valuable reference for making experimental measurements and other relevant researches in the future. Fig. 1 gives the varying regularities of fine structure splittings for $1s^2np$ and $1s^2nd$ states with the increasing of n values.

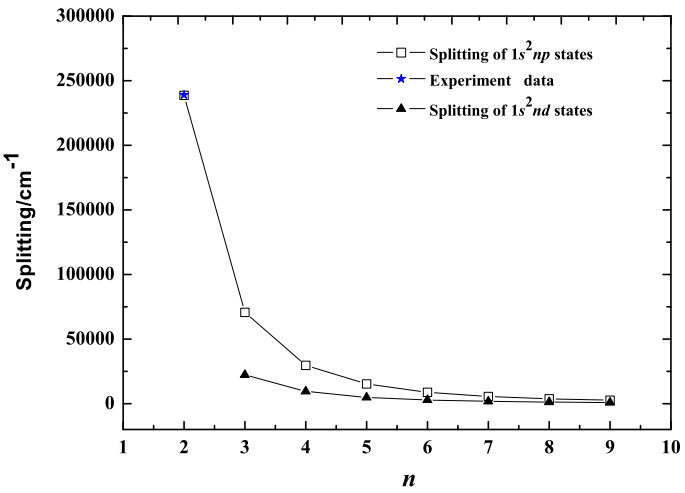

Figure 1: The fine structure splittings of $1s^2np$ and $1s^2nd$ states for Zn^{27+} ion.

In calculating the first-order approximation of the splitting, we not only take account of the spin-orbit interaction, but also consider of the contribution from spin-other-orbit interaction. The contributions from these two effects constitute the greatest part in the total splittings. It is seen from Table 1 that for $1s^2np$ states of the ion, the higher-order relativistic correction gives about 2.5% of the total splittings. For $1s^2nd$ states, the contribution from higher-order relativistic correction is about 0.7% of the total splittings. The contributions from QED effect in the total splittings are about 0.2% for both of $1s^2np$ and $1s^2nd$ states of Zn^{27+} ion.

Table 1: Fine structure splittings for the $1s^2np$ and $1s^2nd$ states of Zn^{27+} ion (in cm^{-1}).

States	S–O + S–O–O	QED corr.	Higher-order rel.	Total splitting	Exp. [9]
$1s^22p$	232114.38	530.24	6041.89	238686.51	239086
$1s^23p$	68622.32	156.22	1844.81	70623.35	
$1s^24p$	28917.29	65.72	752.11	29735.12	
$1s^25p$	14794.42	33.59	370.92	15198.93	
$1s^26p$	8556.76	19.42	207.71	8783.89	
$1s^27p$	5386.23	12.22	127.23	5525.69	
$1s^28p$	3607.19	8.18	83.27	3698.64	
$1s^29p$	2533.24	5.74	57.35	2596.33	
$1s^23d$	22147.21	51.53	161.16	22359.90	
$1s^24d$	9338.85	21.74	76.23	9436.81	
$1s^25d$	4780.40	11.13	39.55	4831.08	
$1s^26d$	2766.06	6.44	22.61	2795.10	
$1s^27d$	1741.74	4.06	13.96	1759.75	
$1s^28d$	1166.73	2.72	9.16	1178.60	
$1s^29d$	817.66	1.91	6.30	825.87	

4 Summary

In this paper, based on calculating the expectation values of the spin-orbit and spin-other-orbit interaction operators with FCPC-type wave functions, the contributions to fine structure splittings for $1s^2np$ and $1s^2nd$ states of Zn^{27+} ion from the higher-order relativistic and QED effects are estimated by introducing the effective nuclear charges. Our result of fine structure splitting in $1s^22p$ state agrees closely with the experimental datum available in the literature. The contributions to the fine structure splittings from the first-order approximation, the higher-order relativistic, and QED correction are quantitatively analyzed. The result shows that the contributions from later two corrections should be not neglectful in the case interested.

Acknowledgments. The authors would like to thank the support by the National Natural Science Foundation of China under Grant No. 11074102.

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