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.

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Key words: Cu^{26+} ion, transition energy and wavelength, oscillator strength

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

Coulomb potential is [11]

$$E_{\text{Dirac}}(Z) = \frac{1}{\alpha^2} \left\{ 1 + \left[\frac{\alpha Z}{n - k + \sqrt{k^2 - \alpha^2 Z^2}} \right]^2 \right\}^{-1/2} - \frac{1}{\alpha^2}, \tag{3}$$

where $k = j + 1/2$ (j is the total angular momentum of the electron). If we only take the $\alpha^2 Z^4$-order contribution, E_{Dirac} can be reduced to

$$E^{(1)}(Z) = -\frac{Z^2}{2n^2} \left\{ 1 + \frac{\alpha^2 Z^2}{n} \left[\frac{1}{k} - \frac{3}{4n} \right] \right\}. \tag{4}$$

Since the energy of nl electron in the system has been calculated to the $\alpha^2 Z^4$-order with Eq. (2), we can define the effective nuclear charge Z_{eff}, affected by nl electron, as

$$E_0(1s^2 nl) + \Delta E_1(1s^2 nl) - E_0(1s^2) - \Delta E_1(1s^2)$$

$$= -\frac{Z_{\text{eff}}^2}{2n^2} \left\{ 1 + \frac{\alpha^2 Z_{\text{eff}}^2}{n} \left[\frac{1}{k} - \frac{3}{4n} \right] \right\}. \tag{5}$$

Using Z_{eff} defined by Eq. (5), the higher-order relativistic contribution can be estimated

$$\Delta E_{\text{higher-order}} = E_{\text{Dirac}}(Z_{\text{eff}}) - E^{(1)}(Z_{\text{eff}}). \tag{6}$$

The ionization potentials (*IP*) of $1s^2 nl$ ($l = s$, and p) states for Cu^{26+} ion are given by the difference between energies of three-electron system and $1s^2$-core. So we can assume that the QED effect of $1s^2$-core is canceled out in the ionization potential of three-electron system. Thus this correction to energy can be evaluated only for the valence electron by using a hydrogenic formula [11] with an effective nuclear charge, Z_{eff}. This correction, ΔE_{QED}, consists of two parts: the shift of the centre-of gravity of energy, ΔE_{QED}^g, for $1s^2 nl$ configuration and the contribution, ΔE_{QED}^J, to the fine-structure splitting of the L^2 systems. Their explicit expressions were given in Ref. [12].

Table 1: The energies of $1s^2 2s$ and $1s^2 np$ ($n \leq 9$) states for Cu^{26+} ion (in a.u.)

States	Non-rel.	1-st corr.	QED corr.	Higher rel.	Total
$1s^2 2s$	-916.87243435	-10.04623602	0.08689360	-0.2530513	-926.85708190
$1s^2 2p$	-914.94373536	-9.31412842	0.07475878	-0.00849860	-924.19160360
$1s^2 3p$	-863.76126410	-9.03402473	0.02203237	-0.00295546	-872.77621192
$1s^2 4p$	-845.90958915	-8.92388791	0.00925779	-0.00127833	-854.82549760
$1s^2 5p$	-837.66136116	-8.87695212	0.00472649	-0.00065096	-846.53423775
$1s^2 6p$	-833.18567239	-8.85423575	0.00272956	-0.00036872	-842.03754730
$1s^2 7s$	-830.48895362	-8.84192984	0.00171621	-0.00022768	-839.32939493
$1s^2 8p$	-828.73964721	-8.83475204	0.00114831	-0.00014967	-837.57340061
$1s^2 9p$	-827.54089742	-8.83027388	0.00080573	-0.00010331	-836.37046888

To sum up, we obtain the *IP* of $1s^2nl$ states for Cu^{26+} ion as follows

$$IP(1s^2nl) = \left[E_0(1s^2) + \Delta E(1s^2)\right] - \left[E_0(1s^2nl^2L) + \Delta E(1s^2nl^2L)\right]$$
$$- \Delta E_{\text{higher}-\text{order}} - \Delta E_{\text{QED}}^g(nl). \tag{7}$$

The transition energies of $1s^22s - 1s^2np$ for this ion are determined by the difference between the *IP*s of the initial and final states.

The dipole oscillator strength is given by any one of the following three forms [13]

$$f_L = \frac{2}{3}(E_j - E_i)\left|\left\langle \Psi_j \left| \sum_i \mathbf{r}_i \right| \Psi_i \right\rangle\right|^2,$$

$$f_V = \frac{2}{3(E_j - E_i)}\left|\left\langle \Psi_j \left| \sum_i \nabla_i \right| \Psi_i \right\rangle\right|^2,$$

$$f_A = \frac{2}{3(E_j - E_i)^3}\left|\left\langle \Psi_j \left| \sum_i \frac{\mathbf{r}_i}{r_i^3} \right| \Psi_i \right\rangle\right|^2. \tag{8}$$

Here E_i and E_j are the energies of initial and final states for the dipole transition, respectively. These three alternatives are called the length, velocity and acceleration forms, respectively. All of them are identical theoretically, but in general give rather different results when approximation wave functions are used [13].

3   Results and discussion

In this work, for the $1s^2$-core wave function we used 222 terms in seven l components. To calculate the non-relativistic energies of $1s^22s$ and $1s^2np$ ($n \leq 9$) states for Cu^{26+} ion, we used nine and ten d_i terms in Eq. (1), respectively. The number of terms in $\Phi_{n(i),l(i)}$ ranges

Table 2: The transition energies (in cm^{-1}) and the wavelengths (in Å) of $1s^22s - 1s^2np$ for Cu^{26+} ion.

Transitions	This work		Experiment [14]	
	Transition energies	Wavelengths	Transition energies	Wavelengths
$1s^22s - 1s^22p$	585000	170.94	582562	171.66
$1s^22s - 1s^23p$	11869277	8.42	11878493	8.42
$1s^22s - 1s^24p$	15808969	6.33	15820697	6.32
$1s^22s - 1s^25p$	17628675	5.67	17641407	5.67
$1s^22s - 1s^26p$	18615576	5.37		
$1s^22s - 1s^27p$	19209942	5.21		
$1s^22s - 1s^28p$	19595335	5.10		
$1s^22s - 1s^29p$	19859346	5.03		

from 680 to 969 terms. Our calculated results of the non-relativistic energies of $1s^2 2s$ and $1s^2 np$ ($n \leq 9$) states are listed in the second column of Table 1. The non-relativistic energies of $1s^2 2s$ and $1s^2 2p$ states obtained in this paper are -916.87243435 a.u. and -914.94373536 a.u., respectively. The corresponding results of Yan *et al* [3] are -916.872436034(70) a.u. and -914.94384214(71) a.u., respectively. The relative discrepancies between them are within 0.1 ppm. It seems to suggest that the non-relativistic energies of $1s^2 2s$ and $1s^2 np$ states obtained in this work are accurate and reliable enough. This table also gives the contributions to energy from the first perturbation of relativistic and mass-polarization effects, QED and higher-order relativistic corrections. They are listed in the third, fourth and fifth columns of the table, respectively. The numbers listed in the last column marked by "Total" in the table represents the total energies of $1s^2 2s$ and $1s^2 np$ states for this ion, which are the summations of non-relativistic energies, first-order corrections, and the contributions from QED and higher-order relativistic corrections. It is noted that the contributions to energy from later two effects should not be neglected for this ion.

Table 2 gives our calculated results of transition energies and wavelengths of $1s^2 2s - 1s^2 np$ ($n \leq 9$) for Cu^{26+} ion, and experimental data [14]. It is found from the table that our results agree closely with experimental data. This shows that our theoretical predictions about $1s^2 2s - 1s^2 np$ ($n = 6, 7, 8,$ and 9) transitions should be accurate enough, although there are not experimental data available in literature yet in these cases.

Table 3: The dipole oscillator strengths for $1s^2 2s - 1s^2 np$ of Cu^{26+} ion.

Transitions	f_L	f_V	f_A	Other theory [3]
$2s - 2p$	0.04643	0.04643	0.04048	0.046427554(14)
$2s - 3p$	0.39103	0.39098	0.39062	
$2s - 4p$	0.09634	0.09623	0.09629	
$2s - 5p$	0.03975	0.03978	0.03977	
$2s - 6p$	0.02062	0.02063	0.02064	
$2s - 7p$	0.01219	0.01216	0.01245	
$2s - 8p$	0.00784	0.00785	0.00785	
$2s - 9p$	0.00536	0.00537	0.00537	

The oscillator strengths, in three forms, of $1s^2 2s - 1s^2 np$ ($n \leq 9$) for Cu^{26+} ion, obtained in this work, are listed in Table 3. For $1s^2 2s - 1s^2 2p$ transition of this ion, the oscillator strength obtained by Yan *et al*. is 0.046427554(14) [3]. Our f-values of length and velocity forms are 0.04643 which agree with the result of Yan *et al* up to four digits. It is seen from Table 3 that the agreement among our f-values in three forms is satisfactory in the most cases. This indicates that our FCPC wave functions of $1s^2 2s$ and $1s^2 np$ ($n \leq 9$) states for Cu^{26+} ion, determined in this work, should be accurate in the whole configuration space from small r to large r. So far as we know, there is not the report on experimental data of oscillator strengths for these transitions of this ion. We hope that our theoretical predictions will be helpful for making experimental measurements in the future.

4 Summary

The non-relativistic energies of $1s^2 2s$ and $1s^2 2p$ states for Cu^{26+} ion obtained in this paper are in excellent agreement with the results of Yan *et al* [3]. By estimating the higher-order relativistic contribution and QED correction to the energy, we have calculated the transition energies and wavelengths of $1s^2 2s - 1s^2 np$ ($n \leq 9$) for this ion. The results agree closely with experimental data available in literature. Our f-value of $1s^2 2s - 1s^2 2p$ transition for this ion agrees with high-precision result [3] up to four digits. The close agreement between the f-values of different gauges indicates the FCPC wave functions determined in this paper should have rather accurate behaviors in the whole configuration space.

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