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RESEARCH ARTICLE

Theoretical study on the $1s^22s$–$1s^2np$ transitions for Ni^{25+} ion

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The transition energies, wavelengths and oscillator strengths for the $1s^22s$–$1s^2np$ ($n \leqslant 9$) transitions of Ni^{25+} ion are calculated. In calculation of the energies, we not only take account of the first-order corrections from relativistic and mass–polarization effects, but also estimate the higher-order relativistic contribution and QED correction by introducing the effective nuclear charge. The results agree with experimental data available in literature satisfactorily. Grotrian diagram showing these transitions is given.

Keywords Ni^{25+} ion, higher-order relativistic contribution and QED corrections, Grotrian diagram, oscillator strength

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1 Introduction

The structures and properties of highly ionized atomic systems are of significant importance for research in many fields, such as laser physics, controlled thermonuclear reactions and astrophysics [1]. In recent years, there have been several reports of calculations of energies and oscillator strengths for lithiumlike ions in literature [2–4]. It should be pointed out, among these work, that Yan *et al.* [3] obtained the high-precision energies and oscillator strengths of $1s^22s$–$1s^22p$ transition for Li-like ions up to $Z = 50$ using Hylleraas-type variational method and the $1/Z$ expansion method. However, for lithiumlike ions with higher Z, particularly for their excited states, there were few data available in literature. Not long ago, we used the full-core plus correlation method, which was developed by Chung [5], to calculate the energy and oscillator strength of Sc^{18+} and V^{20+} ions [6, 7]. But the first-order relativistic correction was only involved in calculation of the energy.

In this paper, the non-relativistic energies of $1s^22s$ and $1s^2np$ ($n \leqslant 9$) states for Ni^{25+} ion are calculated by using the full-core plus correlation (FCPC) method [5]. The first-order corrections to the energy from the relativistic and mass–polarization effects are evaluated with perturbation theory. The higher-order relativistic contribution and QED correction to the energy are estimated by introducing the effective nuclear charge. The transition energies, wavelengths and oscillator strengths of $1s^22s$–$1s^2np$ for this ion are calculated. The results agree well with experimental data available in literature. Grotrian diagram indicating these transitions is given.

2 Theoretical methods

The wave functions of $1s^22s$ and $1s^2np$ states for lithiumlike Ni^{25+} ion are given by

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

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. [5]. The factor multiplying $\Phi_{1s1s}(1, 2)$ is a linear combination of the Slater orbitals for the valence electron. 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) of $1s^22s$ and $1s^2np$ states are calculated with the Rayleigh–Ritz variation method [5]. Their corresponding FCPC wave functions Ψ are determined in this process.

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

$$\Delta E = \Delta E_1 + \Delta E_2 \tag{2}$$

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 the two-particle operators including the electron–electron contact term, orbit–orbit interaction and mass-polarization effect. The expressions of these operators can be found in Ref. [5].

In order to obtain more accurate results for the higher Z system, QED and higher-order relativistic effects on the energy should be involved. As is known, the energy eigenvalue of one-electron Dirac equation (excluding the rest mass energy) for a Coulomb potential is [8]

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

where α is the fine-structure constant, and $k = j + 1/2$ (j is the total angular momentum of the electron). If the $\alpha^2 Z^4$-order contribution is simply retained, 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}, which is affected by nl electron, as

$$\begin{aligned} &E_0(1\text{s}^2nl) + \Delta E_1(1\text{s}^2nl) - E_0(1\text{s}^2) - \Delta E_1(1\text{s}^2) \\ &\quad = -\frac{Z_{\text{eff}}^2}{2\,n^2}\left[1+\frac{\alpha^2 Z_{\text{eff}}^2}{n}\left(\frac{1}{k}-\frac{3}{4n}\right)\right] \end{aligned} \tag{5}$$

The higher-order relativistic contribution can be estimated by

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

In addition, using this Z_{eff} defined in Eq. (5), QED correction to energy can be evaluated with a hydrogenic formula [8]. This correction ΔE_{QED} consists of two parts: the shift of the centre of gravity of energy $\Delta E^{\text{g}}_{\text{QED}}$ for 1s^2nl configuration and the contribution $\Delta E^{\text{J}}_{\text{QED}}$ to the fine-structure splitting of the ^2L systems. Their explicit expressions were given in Ref. [8].

To sum up, we obtain the IP (ionization potential) of 1s^2nl states for Ni^{25+} ion as follows:

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

The transition energies of $1\text{s}^22\text{s}$–$1\text{s}^2n\text{p}$ for this ion are determined in terms of 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 [7, 9]:

$$\begin{aligned} f_L &= \frac{2}{3}(E_j - E_i)\left|\left\langle \Psi_j\right| \sum_i \boldsymbol{r}_i \left|\Psi_i\right\rangle\right|^2 \\ f_V &= \frac{2}{3(E_j - E_i)}\left|\left\langle \Psi_j\right| \sum_i \nabla_i \left|\Psi_i\right\rangle\right|^2 \\ f_A &= \frac{2}{3(E_j - E_i)^3}\left|\left\langle \Psi_j\right| \sum_i \frac{\boldsymbol{r}_i}{r_i^3} \left|\Psi_i\right\rangle\right|^2 \end{aligned} \tag{8}$$

Here Ψ_i and Ψ_j are the wave functions of the initial and final states, and $(E_j - E_i)$ is the transition energy. These three alternative forms are called the length, velocity, and acceleration forms, respectively. They are theoretically equivalent when exact wave functions are used, but usually give rather different results when approximate wave functions are used [9]. According to these formulas, the values of oscillator strength in the three forms can be calculated with the transition energies and wave functions of initial and final states obtained above.

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 $1\text{s}^22\text{s}$ and $1\text{s}^2n\text{p}$ ($n \leqslant 9$) states for Ni^{25+} ion, we used nine d_i terms in Eq. (1). The number of terms in $\Phi_{n(i),l(i)}$ ranges from 638 to 979 terms. For the $1\text{s}^2n\text{p}$ energy calculation, the contribution from the second term on the right-hand side in Eq. (1) rapidly decreases with the increase of principal quantum number. For instance, the contributions are 0.006 804 a.u. and 0.000 111 a.u., respectively, in $1\text{s}^22\text{p}$ and $1\text{s}^29\text{p}$ states.

Our calculated results of the energies of $1\text{s}^22\text{s}$ and $1\text{s}^2n\text{p}$ ($n \leqslant 9$) states for Ni^{25+} ion are listed in Table 1. The non-relativistic energies of $1\text{s}^22\text{s}$ and $1\text{s}^22\text{p}$ states obtained in this paper are −853.770 264 11 a.u. and −851.912 372 19 a.u., respectively. The corresponding results [3] of Yan *et al.* are −853.770 265 374 (72) a.u. and −851.912 462 66 (74) a.u., respectively. The relative discrepancies between them are within 0.1 ppm. This indicates that the non-relativistic energies obtained in this work are accurate and reliable enough. This table also gives the first-order corrections from relativistic and mass–polarization effects, the higher relativistic and QED corrections. The first-order corrections are given by the expectation values of relativistic and mass-polarization perturbation operators. As mentioned above, this part of contributions from relativistic effects

Table 1 The energies of $1s^22s$ and $1s^2np$ states for Ni^{25+} ion (in a.u.).

States	Non-Rel.	1st Corr.	Higher Rel.	QED Corr.	Total
$1s^22s$	−853.770264	−8.70547973	−0.02169191	0.07296111	−862.424475
$1s^22p$	−851.912372	−8.07179089	−0.00722933	0.06286284	−859.928530
$1s^23p$	−804.432733	−7.83108937	−0.00247480	0.01852687	−812.247770
$1s^24p$	−787.874529	−7.73647688	−0.00105848	0.00779558	−795.604269
$1s^25p$	−780.224412	−7.69624744	−0.00053423	0.00398507	−787.917208
$1s^26p$	−776.073431	−7.67664091	−0.00030220	0.00230373	−783.748071
$1s^27p$	−773.572432	−7.66607760	−0.00018611	0.00144962	−781.237246
$1s^28p$	−771.950061	−7.65989209	−0.00012189	0.00097059	−779.609104
$1s^29p$	−770.838246	−7.65605666	−0.00008401	0.00068137	−778.493705

Table 2 The transition energies (in cm^{-1}) and the wavelengths (in Å) of $1s^22s$–$1s^2np$ for Ni^{25+} ion.

Transitions	This work		Experiment [10]	
	Transition energies	Wavelengths	Transition energies	Wavelengths
$1s^22s$–$1s^22p$	547852.75	182.531	545406	183.349
$1s^22s$–$1s^23p$	11012472.66	9.080	11019670	9.074
$1s^22s$–$1s^24p$	14665265.20	6.818	14674533	6.815
$1s^22s$–$1s^25p$	16352364.26	6.115	16362500	6.1115
$1s^22s$–$1s^26p$	17267375.71	5.791		
$1s^22s$–$1s^27p$	17818433.01	5.612		
$1s^22s$–$1s^28p$	18175765.42	5.502		
$1s^22s$–$1s^29p$	18420564.95	5.429		

is merely the α^2Z^4-order contribution. The higher relativistic corrections for $1s^2np$ states listed in the table are the weighted average values of those for the two levels, $^2P_{1/2}$ and $^2P_{3/2}$, obtained from Eq. (6). As indicated in the table, the contributions to the energy from the latter two corrections should not be negligible for this ion, and their contributions decrease monotonously with increasing n-value, as predicted.

Our calculated results of transition energies and wavelengths for $1s^22s$–$1s^2np$ ($n \leqslant 9$) of Ni^{25+} ion are listed in Table 2. Available experimental data [10] are also listed in this table for a comparison. It is found from the table that our results agree well with the experimental data. It seems to have suggested that our theoretical predictions of $1s^22s$–$1s^2np$ ($n = 6$, 7, 8, and 9) transitions should be accurate enough, although there are not experimental data in literature in these cases yet.

A Grotrian diagram showing transitions from ground state $1s^22s$ to $1s^2np$ states of this ion is given in Fig. 1.

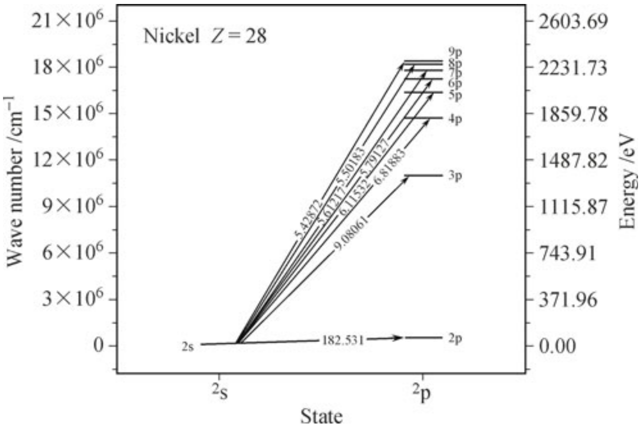

Fig. 1 A Grotrian diagram of $1s^22s$–$1s^2np$ transition for Ni^{25+} ion. Wavelengths are in Å.

Table 3 gives the results of dipole oscillator strengths for $1s^22s$–$1s^2np$ of Ni^{25+} ion. It can be seen that in most cases the obtained f-values in the three forms share a high identity of three or four digits, and our f-values

Table 3 Dipole oscillator strengths for $1s^22s$–$1s^2np$ of Ni^{25+} ion.

Transitions	f_L	f_V	f_A	Experiment [11]	Other theory [3]
2s–2p	0.04818	0.04818	0.04597	0.050	0.048184276(16)
2s–3p	0.38945	0.38945	0.38942	0.383	
2s–4p	0.09599	0.09597	0.09596	0.101	
2s–5p	0.03968	0.03969	0.03968	0.040	
2s–6p	0.02060	0.02060	0.02060	0.0213	
2s–7p	0.01218	0.01218	0.01218	0.0125	
2s–8p	0.00783	0.00784	0.00783		
2s–9p	0.00536	0.00536	0.00536		

also agree with experimental data [11]. Both of our f-values of the length and velocity forms are 0.048 18, and tally with the value of 0.048 184 276 (16) obtained by Yan *et al.* [3] by four digits in the case of $1s^22s$–$1s^22p$ transition. As pointed out in Ref. [9], the velocity form involve derivative of approximate wave functions, and the integrand involved in the acceleration form is weighted toward small r region. Therefore, the degree of agreement between the f-values in these three forms becomes a rigorous judgment for the quality of approximate wave functions used in the calculation. Our results show that FCPC wave functions, which are determined in this paper, should have fairly accurate behaviors in the whole configuration space from small r to large r. It is also seen from Table 3 that the oscillator strengths for $1s^22s$–$1s^2n$p transitions are smoothly decreasing from the 2p state to 9p state. This is because the highly excited $1s^2n$p states spatially overlap a little with the ground state.

4 Summary

Having taken the higher-order relativistic contribution and QED correction to the energy into account, we calculated the transition energies and wavelengths of $1s^22s$–$1s^2n$p ($n \leqslant 9$) for Ni^{25+} ion. Our results agree well with experimental data available in literature. A Grotrian diagram showing these transitions is given. The close agreement between the f-values of different gauges indicates that the FCPC wave functions determined in this paper should have fairly accurate behaviors in the whole configuration space. We hope that the theoretical approach used in this paper can be extended to treatment of the higher Z systems. Based on this, the behaviors, such as the amount of relativistic and QED effects contributions, along the isoelectronic sequence can be determined.

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