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Transition energy and dipole oscillator strength for $1s^2 2p$-$1s^2 nd$ of Cr^{21+} ion*

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The transition energies, wavelengths and dipole oscillator strengths of $1s^2 2p$-$1s^2 nd$ ($3 \leq n \leq 9$) for Cr^{21+} ion are calculated. The fine structure splittings of $1s^2 nd$ ($n \leq 9$) states for this ion are also calculated. In calculating energy, we have estimated the higher-order relativistic contribution under a hydrogenic approximation. The quantum defect of Rydberg series $1s^2 nd$ is determined according to the quantum defect theory. The results obtained in this paper excellently agree with the experimental data available in the literature. Combining the quantum defect theory with the discrete oscillator strengths, the discrete oscillator strengths for the transitions from initial state $1s^2 2p$ to highly excited $1s^2 nd$ states ($n \geq 10$) and the oscillator strength density corresponding to the bound–free transitions are obtained.

Keywords: Cr^{21+} ion, transition energy, fine structure splitting, quantum defect
PACC: 3120A, 3120T, 3270C

1. Introduction

The research on highly ionized atomic systems and highly excited atomic systems has been one of important subjects in atomic physics because the knowledge and basic data about the structure and properties of these systems play an important role in many fields of science and technology, such as plasma physics, laser physics and astrophysics, etc.[1] However, the experimental data on these systems are far from satisfactory at present. In general, one has to rely on reliable theoretical predictions for these basic data as input reference data for other fields.[1,2]

Recently, the full-core plus correlation (FCPC) method[3] has been extended to the systems with higher nuclear charge, and some satisfactory results have been obtained.[4–9] In this paper, we will calculate the transition energies, wavelengths and dipole oscillator strengths of $1s^2 2p$-$1s^2 nd$ ($3 \leq n \leq 9$) for lithium-like Cr^{21+} ion. The fine structure splittings of $1s^2 nd$ ($n \leq 9$) states for this ion will be also evaluated. In order to obtain more accurate and reasonable results, the higher-order relativistic contribution to energy is estimated. By combining with the quantum defect theory (QDT) our theoretical predictions on the energy and oscillator strength for this ion are accurately extrapolated to the whole energy region of the system.

2. Theoretical method

By using the square-integrated Slater-type basis sets[3] the wavefunction of the $1s^2 nl$ states for Cr^{21+} ion is expressed as

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

where A is an antisymmetrization operator. The first term on the right–hand side of Eq.(1) is the product of a predetermined $1s^2$-core wavefunction Φ_{1s1s} (1, 2) and a linear combination of Slater orbitals for the valence electron, and it describes the electron correlation in $1s^2$-core and the effect of valence electron in the three-electron system. The second term is similar to the expansion in terms of basis set in traditional configuration interaction (CI) method, and for describing the relaxation of $1s^2$-core and the other possible correlations in the three-electron system. The expressions of Φ_{1s1s} (1, 2) and $\Phi_{n(i),l(i)}$ (1, 2, 3) in Eq.(1) can be found in Ref.[3]. The non-relativistic energies E_0 of the systems are calculated by minimizing the ex-

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pectation values of their non-relativistic Hamiltonian operators, whose explicit expressions have been given in Ref.[3]. The FCPC wavefunctions Ψ of these states are simultaneously determined in this process. The corrections ΔE to the energy of these states from relativistic and mass-polarization effects are calculated by using the first–order perturbation theory,

$$\begin{aligned}\Delta E =& \langle \Psi | H_1 + H_2 | \Psi \rangle + \langle \Psi | H_3 + H_4 + H_5 | \Psi \rangle \\ =& \Delta E_1 + \Delta E_2, \end{aligned} \tag{2}$$

where ΔE_1 is the first-order corrections to energy 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 explicit expressions of these operators are also given in Ref.[3]. Thus the total energy of the systems is,

$$E_{\rm tot} = E_0 + \Delta E. \tag{3}$$

In order to obtain a more accurate result for this ion with a larger nuclear charge Z, the quantum-electrodynamics (QED) and higher-order relativistic effects on the energy should be included. It is assumed that the QED effects of the $1s^2$ core are cancelled out in the ionization potential (IP) of the three-electron system. Thus, this correction, $\Delta E_{\rm QED}$, can be evaluated for the valence nl electron by using hydrogenic formula[10] with an effective nuclear charge $Z_{\rm eff}$. This correction consists of two parts: the shift, $\Delta E^{\rm g}_{\rm QED}$, of the centre-of-gravity of energy for $1s^2nl$ configuration, and the contribution, $\Delta E^{\rm J}_{\rm QED}$, to the fine structure splitting of the ^2L systems. Their explicit expressions are given in Ref.[11].

The effective nuclear charge $Z_{\rm eff}$ for the valence nl electron is determined by the following way. The energy eigenvalue of the one-electron Dirac equation (excluding the rest mass energy) for a Coulomb potential is[10]

$$\begin{aligned}E_{\rm Dirac}(Z) =& \frac{1}{\alpha^2}\left\{1+\left[\frac{\alpha Z}{n-k+\sqrt{k^2-\alpha^2Z^2}}\right]^2\right\}^{-1/2} \\ & -\frac{1}{\alpha^2}, \end{aligned} \tag{4}$$

where $k = j + 1/2$ (j is the total angular momentum of the hydrogenic electron). To order of α^2Z^4, $E_{\rm Dirac}$ reduces to

$$E^{(1)}(Z) = -\frac{Z^2}{2n^2}\left\{1+\frac{\alpha^2Z^2}{n}\left[\frac{1}{k}-\frac{3}{4n}\right]\right\}. \tag{5}$$

Since the energy of the nl electron has been calculated to order of α^2Z^4 with Eq.(2), we can define a $Z_{\rm eff}$ by

$$\begin{aligned}& E_0(1s^2nl) + \Delta E_1(1s^2nl) - E_0(1s^2) - \Delta E_1(1s^2) \\ =& -\frac{Z^2_{\rm eff}}{2\,n^2}\left\{1+\frac{\alpha^2Z^2_{\rm eff}}{n}\left[\frac{1}{k}-\frac{3}{4n}\right]\right\}. \end{aligned} \tag{6}$$

Using this $Z_{\rm eff}$, an approximate $\Delta E_{\rm QED}$ for the nl electron can be estimated. In addition, we can also use this $Z_{\rm eff}$ to estimate the higher-order relativistic contribution from

$$\Delta E_{\rm higher-order} = E_{\rm Dirac}(Z_{\rm eff}) - E^{(1)}(Z_{\rm eff}). \tag{7}$$

The ionization potential (IP) of $1s^2nl$ state for Cr^{21+} ion is given by

$$\begin{aligned}& {\rm IP}\left(1s^2nl\right) = E_{\rm tot}\left(1s^2\,{}^1S\right) - E_{\rm tot}\left(1s^2nl\,{}^2L\right) \\ & - \Delta E_{\rm higher-order} - \Delta E^{\rm g}_{\rm QED}\left(nl\right). \end{aligned} \tag{8}$$

The transition energy, $E_{\rm tran}$, of $1s^22p$-$1s^2n$d for this ion is determined by the difference between the IPs of two states.

The fine structure splitting for $1s^2n$d states of Cr^{21+} ion is obtained by the summation of the expectation values of the operators for spin-orbit interaction and spin-other-orbit interaction (the explicit expressions of these operators are given in Ref.[11]), and the corresponding QED correction $\Delta E^{\rm J}_{\rm QED}$.

According to QDT,[12,13] the quantum defect μ_n of $1s^2n$d states of Cr^{21+} ion is defined as

$$E_n = -\frac{Z_{\rm c}^2}{2(n-\mu_n)^2}, \qquad \text{(in a.u.)} \tag{9}$$

where$Z_{\rm c} = Z-N+1$ (Z is nuclear charge, and N=3 is the number of electrons in the system), n is principal quantum number, and E_n is the term energy obtained above for $n \le 9$. The quantum defect μ_n for highly excited states should be a smooth function of energy, and can be approximately expanded in the following form

$$\mu_n = \mu_0 + h_1E + h_2E^2, \tag{10}$$

where μ_0 is the quantum defect at the ionization threshold. The coefficients h_1 and h_2 can be determined by using an iteration method. The term energy of any highly excited states $1s^2n$d ($n \ge 10$) for Cr^{21+} ion can be predicted from Eq.(9) and the μ_n value obtained above, as input.

By using the transition energy of $1s^22p$-$1s^2n$d and wavefunctions obtained above, the dipole oscillator strengths in three forms, so called the length, velocity, and acceleration forms, are calculated. The explicit

expressions of these three alternatives were given in Refs.[2, 6].

According to QDT,[12−14] the bound-bound transitions from a given initial state $1s^2 2p$ to any discrete final $1s^2 nd$ states and the bound-continuum transitions from the same initial state to the corresponding continuum states can be treated in a unified form. There is the following relationship between them[15]

$$\tau(E) = \frac{(n*)^3}{Z^2} f_{ij} = \frac{\mathrm{d}f}{\mathrm{d}\varepsilon} = \left(\frac{E_i}{E_i - E_j}\right)^s \left.\frac{\mathrm{d}f}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}, \quad \text{(in a.u.)} \tag{11}$$

where E_i and E_j are the energies of the initial and final states, respectively; $n^* = n - \mu_n$ is the effective quantum number of the final state. The oscillator strength at the threshold, $(\mathrm{d}f/\mathrm{d}\varepsilon|_{\varepsilon=0})$, and s are determined from our predicted discrete oscillator strengths. Thus, the theoretical prediction for this important spectral property of Cr^{21+} ion can be extrapolated to the whole energy region including the continuum states.

3. Results and discussion

The calculated results of transition energies and wavelengths for $1s^2 2p\text{-}1s^2 nd$ ($n \leq 9$) of Cr^{21+} ion are listed in Table 1. It is seen from the table that our results agree excellently with experimental data.[16] The wavelengths of these transitions are in hard x-ray region. This is one of the important properties of highly ionized atomic systems, that differ from those of neutral atoms or lowly ionized atoms. Table 2 gives the values of fine-structure splitting of $1s^2 nd$ ($n \leq 9$) states for Cr^{21+} ion. It is seen from this table that the contribution from higher-order relativistic effect rapidly decreases with increasing principal quantum number for valence electron. Figure 1 shows the variation of the splittings with n. It is clear from Table 2 and Fig.1 that the agreement between our results and experimental data[16] is very satisfactory, and their variation follows a well-behaved regularity of spin-orbit interaction with n in a Rydberg series, which is the main physical factor resulting in fine structure of the term energy.

Table 1. Transition energies and wavelengths of $1s^2 2p\text{-}1s^2 nd$ for Cr^{21+} ion.

Transitions	This work		Exp.[16]	
	$E_{\mathrm{tran}}/\mathrm{cm}^{-1}$	λ/Å	$E_{\mathrm{tran}}/\mathrm{cm}^{-1}$	λ/Å
$1s^2 2p\text{-}1s^2 3d$	7552835	13.2401	7553320	13.239
$1s^2 2p\text{-}1s^2 4d$	10137427	9.8644	10139120	9.863
$1s^2 2p\text{-}1s^2 5d$	11334280	8.8228	11336336	8.821
$1s^2 2p\text{-}1s^2 6d$	11984463	8.3441		
$1s^2 2p\text{-}1s^2 7d$	12376482	8.0798		
$1s^2 2p\text{-}1s^2 8d$	12630892	7.9171		
$1s^2 2p\text{-}1s^2 9d$	12805309	7.8093		

Table 2. Fine structure splittings (in cm^{-1}) of $1s^2 nd$ states for Cr^{21+} ion.

States	Relativistic	QED. corr.	Higher rel.	Total	Exp.[16]
$1s^2 3d$	8418.57	19.64	38.06	8476.27	8480
$1s^2 4d$	3550.79	8.28	17.77	3576.84	3580
$1s^2 5d$	1821.06	4.24	9.09	1834.49	1840
$1s^2 6d$	1053.67	2.45	5.31	1061.43	
$1s^2 7d$	663.46	1.55	3.23	668.24	
$1s^2 8d$	444.44	1.03	2.05	447.52	
$1s^2 9d$	311.42	0.73	1.50	313.65	

The expansion coefficients (see Eq.(10)) of quantum defect μ_n for $1s^2 nd$ series of Cr^{21+} ion are given in Table 3. As a smoothly varying function of energy, the quantum defect μ_n for this series is determined. The ionization energies of $1s^2 nd$ ($6 \leq n \leq 9$) states for Cr^{21+} ion are recalculated by solving Eqs.(9) and (10) with an iteration procedure. The results are listed in the third row marked by 'Semi-Emp' in Table 4. The comparison of these results with the results of our *ab initio* calculation indicates that the relative discrep-

ancy between them is less than 10^{-4}. This shows that the quantum defect μ_n for $1s^2nd$ series of Cr^{21+} ion determined above is reliable, and the energies of any highly excited states ($n \geq 10$) for this series can be accurately predicted.

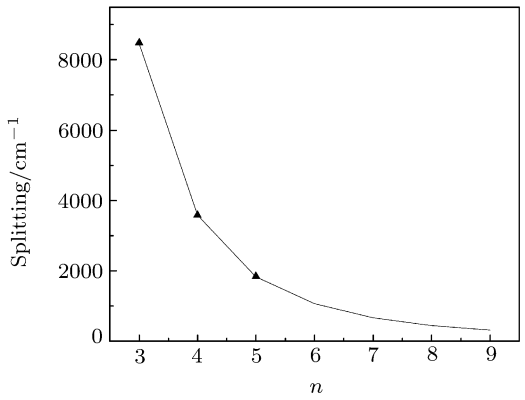


Fig.1. Fine structure splittings of $1s^2nd$ states for Cr^{21+} ion.

Table 3. The coefficients in the expansion of quantum defects for $1s^2nd$ states.

States	μ_0	h_1	h_2
$1s^2nd$	0.004638103	0.0001385305	0.00000136824

Table 4. The comparison of ionization potentials (in a.u.) for $1s^2nd$ ($n \geq 6$) states of Cr^{21+} ion obtained from FCPC method and semi-empirical method.

n	6	7	8	9
FCPC	6.730790	4.944600	3.785414	2.990259
Semi-Emp.	6.732627	4.945327	3.785638	2.990736

Table 5 gives the results of dipole oscillator strengths for $1s^22p$-$1s^2nd$ ($n \leq 9$) of Cr^{21+} ion. As can be seen from this table, the agreement among our f-values in three forms is quite satisfactory, and our calculated results are in close agreement with experimental data.[17] This indicates that our FCPC wavefunctions have a reasonable behaviour over the whole configuration space for Cr^{21+} ion.

Table 5. Dipole oscillator strengths for $1s^22p$-$1s^2nd$ of Cr^{21+} ion.

Transitions	f_L	f_V	f_A	Exp.[17]
2p-3d	0.68151	0.68125	0.68176	0.68
2p-4d	0.12206	0.12203	0.12197	0.12
2p-5d	0.04481	0.04480	0.04477	0.045
2p-6d	0.02124	0.02192	0.02190	0.0220
2p-7d	0.01252	0.01252	0.01251	0.0126
2p-8d	0.00789	0.00790	0.00799	
2p-9d	0.00532	0.00532	0.00536	

Figure 2 depicts dipole transition function (Eq.(11)) of $1s^22p$-$1s^2nd$ for Cr^{21+} ion. It is shown that the discrete oscillator strengths obtained in our calculations follow closely the curve represented by Eq.(11). These and the oscillator strength densities corresponding to bound–free transitions join smoothly across the ionization threshold $E = I$.

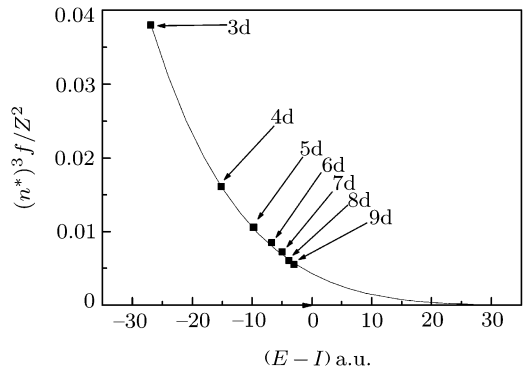


Fig.2. Oscillator strength of $1s^22p$-$1s^2nd$ for Cr^{21+} ion. The full curve is obtained from Eq.(11), and the dots represent the f-values computed in this paper, multiplied by respective factor $(n^*)^3/Z^2$. In Eq.(11), $df/d\varepsilon|_{\varepsilon=0}$= 0.004300, and s=2.924118.

4. Summary

In this paper, we have calculated the transition energies, wavelengths and dipole oscillator strength of $1s^22p$-$1s^2nd$ ($n \leq 9$), and fine structure splittings of $1s^2nd$ states for Cr^{21+} ion. In calculation of energy, the higher-order relativistic contribution is estimated. The quantum defect of $1s^2nd$ series, as a function of energy, is determined; it provides a reliable physical basis for predicting the energies of any highly excited states for this series below the ionization limit. The f-values of three alternative forms agree well with one another. These calculated results excellently agree with experimental data available in the literature. By combining with QDT, the theoretical predictions of dipole oscillator strengths from given initial state $1s^22p$ to $1s^2nd$ states for Cr^{21+} ion have been extrapolated to the whole energy range including continuum states. We hope that the results in this paper will provide a valuable reference for other researches in the future.

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