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Transition energy and oscillator strength of Sc^{18+} ion*

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The transition energies and the dipole oscillator strengths for the $1s^22s$–$1s^2np$ ($2 \leq n \leq 9$) and $1s^22p$–$1s^2nd$ ($3 \leq n \leq 9$) of lithium-like Sc^{18+} ion are calculated by using the full core plus correlation method. The fine structure splittings of $1s^2np$ and $1s^2nd$ ($n \leq 9$) states are determined from the expectation values of spin-orbit and spin-other-orbit interaction operators. The quantum defects of these series, as function of principal quantum number n, are obtained. The agreement between the f-values obtained from three alternative formulae is excellent. Comparisons of our results with experimental data available in the literature are carried out. Combining the single-channel quantum defect theory with the discrete oscillator strengths obtained in this work, this paper obtains the behaviour of discrete oscillator strengths and oscillator strength densities corresponding to the bound-free transitions adjacent to ionization threshold.

Keywords: Sc^{18+} ion, transition energy, fine structure, oscillator strength
PACC: 3130, 3270C, 3110

1. Introduction

Recently, an increasing amount of effort has been devoted to theoretical prediction of accurate transition rates in highly charged atomic systems, because the quantities play a dominant role in controlled thermonuclear reactions where atomic radiation is the primary energy loss mechanism, in astrophysical study for the knowledge of atomic abundance and in plasma modelling.[1] However, the experimental data of these ions available in the literature are far from satisfactory. Thus the reliable theoretical prediction for these important data is obviously of significance.

From the theoretical point of view, lithium-like systems have been frequently chosen as a test for checking the validity of new theoretical methods. In recent years, some accurate calculations of low-lying excited states for lithium-like systems have been carried out. For instance, King calculated the energies of some low-lying excited ^{2}S states for the lithium isoelectronic series from Z=3 to 10 by using large Hylleraas basis sets.[2] Yan *et al* used Hylleraas-type variational method to calculate the energies of $1s^22s$ ^{2}S and $1s^22p$ ^{2}P states and the oscillator strengths for the $1s^22s$ ^{2}S-$1s^22p$ ^{2}P transitions for the lithium isoelectronic sequences up to Z=20.[3]

An elegant and complete variation approach, namely the full core plus correlation (FCPC) method, has been developed by Chung.[4] This method has been successfully applied to the atomic systems with a $1s^2$-core.[4–8] In the FCPC method, a large predetermined multi-configuration interaction (CI) $1s^2$-core wavefunction is used as a single term in the total wavefunction of three-electron system. The effect of the valence electron is accounted for by multiplying the core wavefunction with a linear combination of single-particle Slater orbitals. The relaxation of the core and other possible correlations are described by another large CI wavefunction. Many elaborate calculations for the dipole polarizabilities,[9] the quadrupole and octupole polarizabilities,[10] the total atomic scattering factors[11] and the hyperfine structure[12] of lithium isoelectronic sequence ($Z \leq 20$) have been carried out. Not long ago, this method was also applied to the excited states $1s^2nl$ (l=s, d and

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f, $n \leq 5$) of lithium-like systems with Z=3 to 20[13] and the ground states of the systems with Z=21 to 30.[14] Lately, this method was used to calculate the energy and fine structure of $1s^2np$ states,[15] the dipole oscillator strengths for $1s^22p$–$1s^2nd$ and $1s^23d$–$1s^2nf$ ($n \leq 9$) transitions of lithium-like systems with Z=11 to 20,[16,17] and the d–f intervals for the lithium Rydberg states.[18] A natural extension is to test this method on the system with higher nuclear charge and in the higher energy region.

In this paper, we calculate the transition energies and the dipole oscillator strengths for $1s^22s$–$1s^2np$ and $1s^22p$–$1s^2nd$ ($n \leq 9$) transitions of lithium-like Sc^{18+} ion (Z=21). Combining these calculated results of discrete oscillator strengths with the single-channel quantum defect theory (QDT), we predict the discrete oscillator strengths for $1s^22s$–$1s^2np$ and $1s^22p$–$1s^2nd$ ($n \geq 10$) transitions and the oscillator strength densities corresponding to the bound-free transitions. The fine structure splittings of $1s^2np$ and $1s^2nd$ states for this ion are determined from the expectation values of spin-orbit and spin-other-orbit interactions operators.

The theoretical method of the present work follows closely that of Ref.[4]. These presentations will not be repeated. In Section 2 the computation in this papers is presented. The calculated results and discussion are given in Section 3. A conclusion is given in Section 4.

2. Computation

The wavefunction of the $1s^2nl$ (l= s, p, and d) state for lithium-like Sc^{18+} ion is given by

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

where A is an anti-symmetrization operator. Φ_{1s1s} (1, 2) is a predetermined $1s^2$ core wavefunction, and its expression can be found in Ref.[4]. The second term on the right-hand side of Eq.(1) describes the relaxation of the $1s^2$ core and the other possible correlations. $\Phi_{n(i),l(i)}$ is the basis set of three electron system.[4,6–8]

The non-relativistic energies (upper bounds) of the $1s^2$ core and the $1s^2nl$ (l= s, p, and d; $n \leq 9$) states are calculated by minimizing the expectation value of the non-relativistic Hamiltonian whose explicit expression is given in Ref.[4]. The relativistic effects, including the correction to kinetic energy, Darwin term, the electron–electron contact term, the orbit–orbit interaction, and mass-polarization effect on the energies are calculated by using the first-order perturbation theory. The explicit expressions of these operators are given in Ref.[4]; they will not be repeated here. In order to obtain a more accurate result for the larger Z system, the quantum-electrodynamics (QED) correction should be included. We assume that the QED effects of the core cancel out in the ionization potential (IP). Thus, this correction to energy can be evaluated for the valence electron by using a hydrogenic formula[19] with an effective nuclear charge, $Z_{\rm eff}$,

$$\begin{aligned}\Delta E_{\rm QED} =& \frac{4Z_{\rm eff}^4}{n^3}\frac{\alpha^3}{3\pi}\left\{\delta_{l,0}\left[\ln\left(Z_{\rm eff}\alpha\right)^{-2} + \frac{11}{24} - \frac{1}{5}\right]\right. \\ & \left. - \ln\left[\frac{K_0\left(nl\right)}{Z_{\rm eff}^2 R_\infty}\right] + \frac{3}{8}\frac{C_{l\,J}}{\left(2l+1\right)}\right\} \\ =& \Delta E_{\rm QED}^J(nl) + \Delta E_{\rm QED}^{\rm g}(nl), \end{aligned} \quad (2)$$

where n is the principal quantum number, R_∞ is the Rydberg constant, α is the fine structure constant and $C_{Jl} = \delta_{J,l+1/2}/(l+1)$-$\delta_{J,l-1/2}/\ l\ $. The first term of Eq.(2) contributes to the splitting of the ^2L (L=P or D) systems, and the second term causes a shift of the centre of gravity for $1s^2nl$ configuration energy. The $Z_{\rm eff}$ is defined by

$$E_{\rm non-rel}(1s^2nl) - E_{\rm non-rel}(1s^2) = -\frac{Z_{\rm eff}^3}{2n^2}. \quad (3)$$

The values of the Bethe logarithms K_0 (nl) are taken from Ref.[20].

The transition energies for $1s^22s$–$1s^2np$ ($2 \leq n \leq 9$) are obtained from the difference between the ionization potential of $1s^22s$ state and that of $1s^2np$ states, namely

$$E_{\rm transition} = E_{\rm IP}\left(1s^22s\right) - E_{\rm IP}\left(1s^2np\right). \quad (4)$$

We have a similar expression for the $1s^22p$–$1s^2nd$ (3 $\leq n \leq 9$) transitions.

For the $1s^2nl$ (l= p and d) states, the fine structures splittings mainly come from the spin–orbit and spin–other-orbit interactions. To calculate the splitting, the LSJ-coupling scheme is used and the result is given by the summation of the expectation values of $H_{\rm SO}$ and $H_{\rm SOO}$ and the QED contribution to the splitting, namely

$$\begin{aligned}\Delta E_{\rm FS}^J =& \langle {\rm LSJM}_J|\ H_{\rm SO} + H_{\rm SOO}\ |{\rm LSJM}_J\rangle \\ & + \Delta E_{\rm QED}^J\left(nl\right), \end{aligned} \quad (5)$$

where the expressions of operators $H_{\rm SO}$ and $H_{\rm SOO}$ can be found from Refs.[7, 8].

According to the single channel quantum defect theory,[21−23] the quantum defect μ_n of the $1s^2nl$ state is defined by the equation

$$E_n = -\frac{Z^2}{2\left(n-\mu_n\right)^2} \quad \text{(in a.u.)}, \tag{6}$$

where n is the principal quantum number, and E_n is the term energy obtained above for $n \leq 9$. For highly excited states, quantum defect μ_n should be a smooth function of energy. So it can be approximated in terms of a weakly varying function of energy in the following form:

$$\mu_n = \mu_0 + h_1 E + h_2 E^2. \tag{7}$$

The coefficients μ_0, h_1, and h_2 for each Rydberg series are determined by using the μ_n values obtained from Eq.(6). Treating Eqs.(6) and (7) as a set of equations for E_n and μ_n, by an iteration method we determine the quantum defect μ_n and term energy E_n for highly excited states ($n \geq 10$). Firstly, we set $\mu_n \approx \mu_0$, and put it into Eq.(6). Then E_n and μ_n can be refined by iteration procedure. Finally, the quantum defect μ_n and the term energy E_n are obtained.

It can be shown that the dipole oscillator strength is given by any of the following three forms:[22]

$$f_{\mathrm{L}} = \frac{2}{3}\left(E_j - E_i\right) \left| \left\langle \Psi_i \right| \boldsymbol{r} \left| \Psi_j \right\rangle \right|^2, \tag{8a}$$

$$f_{\mathrm{V}} = \frac{2}{3}\left(E_j - E_i\right)^{-1} \left| \left\langle \Psi_i \right| \nabla \left| \Psi_j \right\rangle \right|^2, \tag{8d}$$

$$f_{\mathrm{A}} = \frac{2}{3}\left(E_j - E_i\right)^{-3} \left| \left\langle \Psi_i \right| \frac{\boldsymbol{r}}{r^3} \left| \Psi_j \right\rangle \right|^2. \tag{8c}$$

Here $(E_j - E_i)$ is the transition energy. These three alternatives are called respectively the length, velocity and acceleration forms. They should be calculated by summing over the final states and averaging over the initial states. All of them are equivalent when exact wavefunctions are used. But they usually give rather different results when approximate wavefunctions are used, because the matrix elements in these three forms are weighted towards different regions of electron configuration space. Therefore, whether the f-values obtained from the three formulae are in agreement with each other, this is a rigorous evaluation of the quality of the wavefunctions for the initial and final states used in the calculation.

As is known, the oscillator strength densities corresponding to the final states in the continuum are associated with the discrete oscillator strengths corresponding to the bound–bound transitions.[21,22] We can define the oscillator strength densities of the bound–bound transition as

$$\tau\left(E\right) = \frac{\left(n^*\right)^3}{Z^2} f_{ij} \qquad \text{(in a.u.)}, \tag{9}$$

where Z is the charge of the ion core, E is the energy of the final state, and f_{ij} is the discrete oscillator strength. n^* is the effective principal quantum number of the final state, which is given by

$$n^* = n - \mu_n. \tag{10}$$

In the limit $E \to I$ (from below), where I is the ionization potential of the system, $\tau(E)$, as a function of E, will match to the oscillator strength densities, $\mathrm{d}f/\mathrm{d}\varepsilon$ of continuum states, namely

$$\tau\left(E\right) = \frac{\left(n^*\right)^3}{Z^2} f_{ij} = \frac{\mathrm{d}f}{\mathrm{d}\varepsilon}. \tag{11}$$

For the $1s^22s$–$1s^2np$ and $1s^22p$–$1s^2nd$ transitions of lithium-like ion under consideration, neither the Cooper minimum nor the following maximum is found in the near-threshold energy region. Hence, Eq.(11) can be used to extrapolate the discrete oscillator strength f_{ij} below the threshold to the discrete oscillator strength densities $\mathrm{d}f/\mathrm{d}\varepsilon$ above the threshold. In the near-threshold region ($|E| \leq I/2$), the oscillator strength and the oscillator strength densities can be accurately approximated by the following equation:[24]

$$\tau\left(E\right) = \frac{\left(n^*\right)^3}{Z^2} f_{ij} = \frac{\mathrm{d}f}{\mathrm{d}\varepsilon} = \left(\frac{E_i}{E_i - E_j}\right)^S \left.\frac{\mathrm{d}f}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}, \tag{12}$$

where s and the oscillator strength density, $\left.\mathrm{d}f/\mathrm{d}\varepsilon\right|_{\varepsilon=0}$, can be determined from our predicted discrete oscillator strengths. Eqs.(9) and (12) make it possible to determine the oscillator strengths easily for transition from a certain initial state to all the final states of the Rydberg series.

3. Results and discussion

For the $1s^2$-core wavefunction we used 222 terms in seven l components. To calculate the $1s^2nl$ energy, we used eight d_i terms. The number of terms in $\Phi_{n(i),l(i)}$ ranges from about 900 to 1000 terms. Numerical calculations of energies converge rather fast.

Our calculated results of the transition energies for $1s^22s$–$1s^2np$ and $1s^22p$–$1s^2nd$ ($n \leq 9$) of Sc^{18+} ion, and the experimental data available in the literature[25] are listed in Table 1. It is noted that the uncertainties quoted in these experiments are very large. For example, the error bar of these experimental data is in about 10^3–10^4 cm^{-1} for $1s^2np$ states,

and about $10^2 cm^{-1}$ for $1s^2nd$ states. To sum up the comparison between our predicted transition energies and the available experimental data, it is found that our results agree well with theirs and are all within the experimental uncertainties. No experimental data are available for $1s^22s–1s^2np$ (n= 8 and 9) and $1s^22p–1s^2nd$ (n= 9) transitions. We hope our theoretical results may stimulate some interest in making higher precision experimental measurements.

Table 1. The transition energies (in cm^{-1}) for $1s^22s–1s^2np$ and $1s^22p–1s^2nd$ of Sc^{18+} ion.

Transitions	This work	Exp.[25]	Transitions	This work	Exp.[25]
$1s^22s–1s^22p$	344 090	340 500	$1s^22p–1s^23d$	5 637 481	5 639 900
$1s^22s–1s^23p$	5 941 569	5 941 000	$1s^22p–1s^24d$	7 565 010	7 569 100
$1s^22s–1s^24p$	7 892 443	7 890 000	$1s^22p–1s^25d$	8 457 488	8 459 500
$1s^22s–1s^25p$	8 793 109	8 790 000	$1s^22p–1s^26d$	8 942 307	8 942 500
$1s^22s–1s^26p$	9 281 514	9 272 000	$1s^22p–1s^27d$	9 234 621	9 237 500
$1s^22s–1s^27p$	9 575 629	9 576 000	$1s^22p–1s^28d$	9 424 328	9 423 500
$1s^22s–1s^28p$	9 766 366		$1s^22p–1s^29d$	9 554 391	
$1s^22s–1s^29p$	9 897 040				

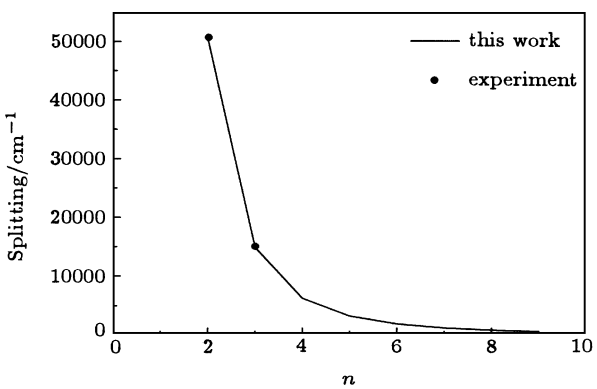


Fig.1. The fine structure splitting for $1s^2np$ ($n \leq$ 9) states of Sc^{18+} ion. Experimental data are from Ref.[25].

According to Eq.(5), our obtained fine structure splittings for $1s^2np$ and $1s^2nd$ ($n \leq$9) states of Sc^{18+} ion are listed in Table 2. Their variations with principal quantum number n are shown in Figures 1 and 2 respectively. It is seen from Table 2 that the error bar in the experimental data available in the literature[25] is quite large, and even in many cases we are not aware of any experimental results for a comparison with theory. It can be seen from Figures 1 and 2 that with the increase of n, our results of the splittings for $1s^2np$ and $1s^2nd$ ($n \leq 9$) states of Sc^{18+} ion follow a well-behaved variation regularity of spin–orbit interaction with n, which is main physical reason leading to fine structure splitting, along a Rydberg series.[22]

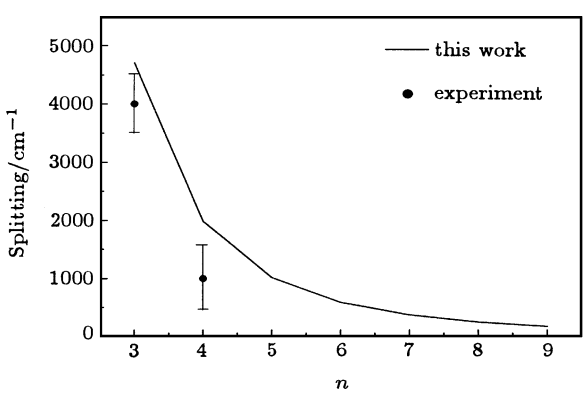


Fig.2. The fine structures splitting for $1s^2nd$ ($n \leq 9$) states of Sc^{18+} ion. Experimental data are from Ref. [25].

Table 2. Fine structure splittings (in cm^{-1}) for $1s^2np$ and $1s^2nd$ states of Sc^{18+} ion.

States	Relativistic	QED corr.	Total	Exp.[25]
$1s^2 2p$	49 898.10	113.20	50 011.30	50 700
$1s^2 3p$	14 740.00	33.27	14 773.27	15 000
$1s^2 4p$	6 208.38	13.98	6 222.36	
$1s^2 5p$	3 175.22	7.14	3 182.36	
$1s^2 6p$	1 836.05	4.13	1 840.18	
$1s^2 7p$	1 155.57	2.60	1 158.17	
$1s^2 8p$	773.71	1.74	775.45	
$1s^2 9p$	543.41	1.22	544.63	
$1s^2 3d$	4 693.72	10.93	4 704.65	4 000
$1s^2 4d$	1 978.71	4.61	1 983.32	1 000
$1s^2 5d$	1 012.76	2.36	1 015.12	
$1s^2 6d$	585.97	1.37	587.34	
$1s^2 7d$	368.96	0.86	369.82	
$1s^2 8d$	247.18	0.58	247.76	
$1s^2 9d$	173.28	0.40	173.68	

According to the procedure of determining quantum defect in the previous section, our obtained expansion coefficients in Eq.(7) are given in Table 3. Thus, the quantum defects μ_n of these two series, $1s^2np$ and $1s^2nd$, of Sc^{18+} ion, as smoothly varying functions of energy, are determined. With these μ_n values as input, the ionization potentials of $1s^2np$ and $1s^2nd$ ($n \leq 9$) states for Sc^{18+} ion are calculated by using the iteration method described in previous section. The results are given in the third column marked by "Semi-empirical" of Table 4. Corresponding results from FCPC method are also listed in this table for a comparison. It is seen that the agreement of them is quite good. We have reason to believe that the quantum defects of these two series determined in this work are reliable, and the energies of any discrete states ($n \geq 10$) of these two series for Sc^{18+} ion below the ionization limit can be accurately predicted by using their quantum defects μ_n as input.

Table 3. The coefficients in the expansion Eq.(7) of the quantum defects.

States	μ_0	h_1	h_2
$1s^2np$ ($2 \leq n \leq 9$)	$1.668\ 516\times10^{-2}$	$-9.020\ 368\times10^{-5}$	$6.932\ 105\times10^{-7}$
$1s^2nd$ ($3 \leq n \leq 9$)	$3.850\ 274\times10^{-3}$	$-1.539\ 613\times10^{-4}$	$2.146\ 294\times10^{-6}$

Table 4. The comparison between the values of ionization potentials (in a.u.) of Sc^{18+} ion obtained from the FCPC method and semi- empirical method.

States	FCPC	Semi-empirical
$1s^2 5p$	7.266 822	7.266 624
6p	5.041 461	5.041 155
7p	3.701 360	3.700 953
8p	2.832 286	2.831 936
9p	2.236 883	2.236 582
$1s^2 6d$	5.019 212	5.019 127
7d	3.687 315	3.687 161
8d	2.822 936	2.822 734
9d	2.230 318	2.230 138

The calculated results of the oscillator strengths for the $1s^2 2s$–$1s^2 np$ ($2 \leq n \leq 9$), $1s^2 2p$–$1s^2 nd$ ($3 \leq n \leq 9$) transitions of lithium-like Sc^{18+} ion are given in Table 5. The experimental data[26,27] available in the literature are also listed in the table. As can be seen from this table, the agreement between our f-values

obtained from the length- and velocity-formulae is up to four digits, and the agreement of our calculated results with experimental data is also fairly satisfactory. The f-values from the acceleration-formula are closely in agreement with them too. The results for the oscillator strengths in this work show that our FCPC wavefunctions have a reasonable behaviour over the whole configuration space of lithium-like Sc^{18+} ion.

Table 5. The dipole oscillator strengths for $1s^22s$–$1s^2np$ and $1s^22p$–$1s^2nd$ transitions of Sc^{18+} ion.

Transitions	f_L	f_V	f_A	Exp.
2s–2p	0.065 55	0.065 54	0.058 83	0.069[a]
2s–3p	0.373 75	0.373 72	0.373 83	0.367[a]
2s–4p	0.093 47	0.093 47	0.093 45	0.098[a]
2s–5p	0.038 85	0.038 85	0.038 85	0.040[a]
2s–6p	0.020 21	0.020 21	0.020 20	0.021 1[a]
2s–7p	0.011 96	0.011 96	0.011 97	0.012 4[a]
2s–8p	0.007 701	0.007 702	0.007 701	0.007 545[b]
2s–9p	0.005 272	0.005 272	0.005 269	
2p–3d	0.679 56	0.679 39	0.680 53	0.68[a]
2p–4d	0.122 11	0.122 11	0.122 07	0.12[a]
2p–5d	0.044 88	0.044 88	0.044 84	0.045 2[a]
2p–6d	0.021 97	0.021 97	0.021 95	0.022 0[a]
2p–7d	0.012 55	0.012 55	0.012 54	0.012 7[a]
2p–8d	0.007 907	0.007 908	0.007 899	0.007 895[b]
2p–9d	0.005 330	0.005 330	0.005 306	

[a] Ref.[26]. [b] Ref.[27].

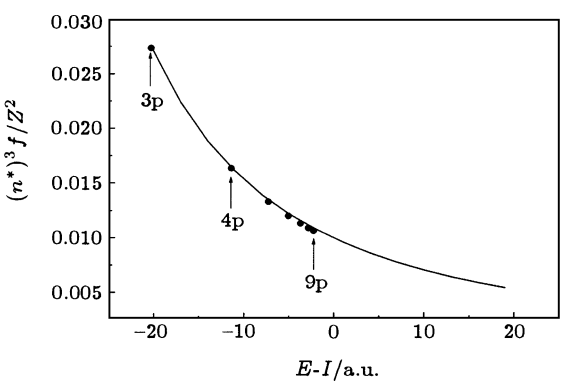


Fig.3. The dipole oscillator strengths for the $1s^22s$–$1s^2np$ transitions of Sc^{18+} ion. The curve is obtained from Eq.(12), and the dots represent the values calculated from Eq.(9). The discrete oscillator strengths are multiplied by factors $(n^*)^3/Z^2$. In Eq.(12),s=1.829713, $\mathrm{d}f/\mathrm{d}\varepsilon|_{\varepsilon=0}$=0.009906295.

The oscillator strengths for transitions from a certain initial state to all states for the Rydberg series are determined by using Eqs.(9) and (12). Figures 3 and 4 depict Eq.(12) corresponding to the $1s^22s$–$1s^2np$ and $1s^22p$–$1s^2nd$ transitions of Sc^{18+}ion, respectively. It is shown that the discrete oscillator strengths calculated from the transition energies and FCPC wavefunctions obtained above lie rather well along the curves expressed by Eq.(12), and these discrete oscillator strengths and the oscillator strength densities corresponding to the bound–free transitions join smoothly across the ionization threshold $E = I$. These results indicate that our extrapolation results are reliable and accurate.

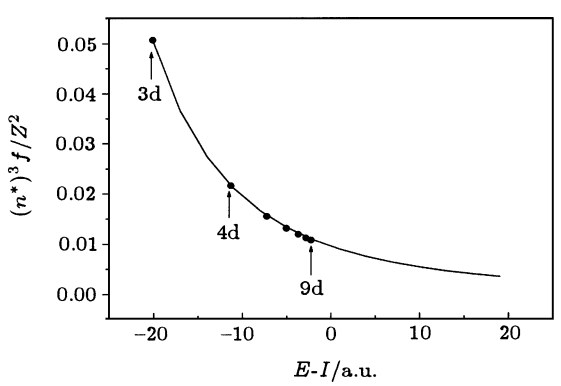


Fig.4. The dipole oscillator strengths for $1s^22p$–$1s^2nd$ transitions of Sc^{18+} ion. The curve is obtained from Eq.(12), and the dots represent the values calculated from Eq. (9). The discrete oscillator strengths are multiplied by factors $(n^*)^3/Z^2$. In Eq.(12), s=2.902559, $\mathrm{d}f/\mathrm{d}\varepsilon|_{\varepsilon=0}$=0.009492251.

4. Conclusion

In this paper, we have calculated the structure

and spectral property in the whole energy region, from discrete states to continuum states, for lithium-like Sc^{18+} ion by combining the FCPC method with QDT. The comparisons of our obtained transition energies of $1s^22s–1s^2np$ and $1s^22p–1s^2nd$ ($n \leq 9$) for Sc^{18+} ion with the experimental data available in the literature indicate that our results should be reliable. Our evaluated fine structure splittings of $1s^2np$ and $1s^2nd$ ($n \leq 9$) states for Sc^{18+} ion follow a well-behaved regularity. By using our determined quantum defects, as function of energy, the energies of any highly-excited states ($n \geq 10$) of these two series for Sc^{18+} ion below the ionization limit can be accurately predicted. The agreement between the values of oscillator strength obtained from the length-, velocity-, and acceleration-formulae shows that our FCPC wavefunctions should be accurate in the whole configuration space, and the predicted f-values should also be accurate. Combining the f-values with quantum defect theory, we have obtained reliable and accurate oscillator strengths for dipole transitions from the given initial states to all the states of these two Rydberg series, including the oscillator strength densities corresponding to bound-free transitions. The results of this paper will provide valuable reference for other researches in future.

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