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Calculations for Spin-allowed Transitions Between Energy Levels Above the 3s3p State in Si III

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Spin-allowed transition probabilities between energy levels above the 3s3p state of Si III are reported by employing a coupled equation within WBEPM theory. The results show a good agreement with critical values, with the derivations mostly less than 15%. The method can readily be applied to highly excited states without any extra effort.

Key words: Transition probability, Si III, WBEPM theory

I. INTRODUCTION

In recent years, much work has been devoted to the calculation of atomic transition probabilities. Interest has been stimulated not only by the practical need to estimate oscillator strengths in such fields as astrophysics, plasma physics, and space research, but also by the fact that transition probabilities provide a quite sensitive measure of the reliability of approximate solutions to the multi-electron problem of atomic structure [1]. The weakest bound electron potential model (WBEPM) theory was presented by one of the authors of this paper in the 1980s, based on which many atomic properties including transitions [2], energy level [3], and ionization [4] have been reported with satisfactory accuracy. In the present work, we will concentrate on spin-allowed transitions between energy levels above the 3s3p state of Si III.

Elements of the Mg I sequence are abundant in the solar corona [5] and emission lines from Mg-like ions are frequently observed in the spectra of astrophysical plasmas [6]. The electron configuration of Mg I sequence is [Ne]$3s^2$. Since there are two valence electrons outside of a closed core. The correlations play an important role in the theoretical calculation. And the reliability of different theoretical schemes can be tested by comparison with measurements of transition rates in fine-structure levels. In the past, much research has been done on the Mg I sequence. Most of the earlier theoretical and experimental work has concentrated on bound-bound transitions linking low-lying levels. The effects of electron correlation in the valence shell must be taken into account in order to obtain reliable transition rates and oscillator strength values in the Mg I sequence. The f-values for ions of the magnesium isoelectronic sequence was calculated by Butler *et al.* as part of the international Opacity Project [7]. The quantum defect orbital (QDO) method has been adopted to evaluate oscillator strengths for transitions involving the principal spectral series in the Mg I sequence by Martin and coworkers [8]. Hong-Binh used the Coulomb approximation (CA) to obtain multiplet oscillator strengths for excited atomic magnesium[9]. Fischer used the multiconfiguration Hartree-Fock (MCHF) approach to study spin-forbidden and spin-allowed transitions in Mg-like ions [10]. Recently, many-body perturbation theory (MBPT) was used by Safronova *et al.* to study transition and lifetimes for electronic transition in Mg sequence [11] and CIV3 computer code was used by Neerja *et al.* to calculate the transition probabilities in Mg-like P IV[12].

Si III, as a member of the Mg sequence, is of particular astrophysical importance in hot stars. Up to now, many studies of transitions in Si III have been performed using a variety of methods. Experimentally, there have been the beam-foil technique [13-17], radio-frequency ion trap [18], and dual-laser-produced plasma (DLP) photoabsorption technique [19]. On the theoretical side, Zare [1] and Weiss [20] performed independent calculations on absolute multiplet strengths for electric dipole transitions in Si III, taking configuration interaction between valence electrons into account. In addition to the fact that both results are well confirmed by each other, the latter shows a better equivalence between the length expression and the velocity one. Moreover, there has also been much work carried out using other methods such as relativistic random-phase approximation (RRPA) [21], multiconfiguration relativistic random-phase approximation (MCRRPA) method [22], configuration interaction (CI) technique [5,6,23,24], R-matrix method [25], multiconfiguration Dirac-Fock (MCDF) method [26,27], multiconfiguration interaction Dirac-Hartree-Fock (MCDHF) [28], multiconfiguration optimized potential model (MCOPM) [29], Time-dependent Hartree-Fock (TDHF) scheme [30], and relativistic multiconfiguration Hartree-Fock (RMCHF) technique [31].

Most of these theoretical studies concentrated on

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$3s^2\ ^1S_0$-$3s3p\ ^1P^0_1$, $^3P^0_{0,1,2}$ transitions [22,24,26-28,31]. Despite of the fact that the resonance transitions are of great importance in practical application, the computational difficulty associated with these methods serves as a reason for the calculations not being extended to higher states. It is well known, regarding these *ab initio* methods, that the accuracy of the results relies to a great extent on the number of the configurations. To achieve good accuracy in practice, it is usually necessary to take into account a large number of configurations. On the other hand, the number of possible configuration functions increases rapidly as the system considered becomes larger, which consequently makes the work tedious and sometimes even impractical. Another fact is that although many studies have been reported, discrepancies exist not only between theory and experiment but also among various experiments as well as various theories. By the beam-foil technique, for instance, the value of the lifetime of the $4f\ ^3F^0$ level given by Irwin *et al.* [17] is less than one-half of the value reported by Berry *et al.* [14]. Shorer *et al.* [21] performed an RRPA calculation for the $3s^2\ ^1S_0$ - $3s3p\ ^1P^0_1$, $3s^2\ ^1S_0$ - $3s4p\ ^1P^0_1$, and $3s^2\ ^1S_0$ - $3s5p\ ^1P^0_1$ transitions. The results of oscillator strength for $3s^2\ ^1S_0$ - $3s3p\ ^1P^0_1$ transition show a fairly good agreement with the experimental data given by Wiese *et al.* [32] and another theoretical value [30], while great discrepancies occur when the results for $3s^2\ ^1S_0$ - $3s4p\ ^1P^0_1$ and $3s^2\ ^1S_0$ - $3s5p\ ^1P^0_1$ are compared with those from Victor *et al.* [33]. These comparisons are available from Table I, II and III in Ref.[21]. As for transitions between excited states, if any, the techniques are limited only to lower states with n<5. This is far from insufficient for practical applications. With this in consideration, further studies on these transitions, especially those between highly excited states, are of great necessity.

We have calculated oscillator strengths and transition probabilities for 3s3p-3s3d, 3s3d-3s4p, 3s4s-3s4p, 3s3d-3s4f, and 3s4d-3s4f transitions in Mg-like ions PIV–ArVII evaluated by WBEPM method [34]. In this work a coupled equation is used to determine the parameters Z' and d is derived by rationally separating the electrons considering their different behaviors in the system, then calculations for transition probabilities between excited states and oscillator strength of Si III were carried out using the WBEPM theory. In order to find out the regulation of the Mg I sequence, the results was associated with our previous work [34]. our data was also compared with those from other methods, to verify the validation and applicability of our theory. Obviously, we can see a prevalent agreement between not only the previous work but also other work of different methods, and the discrepancies between critical values are mostly less than15%.

II. THEORY

Details about the WBEPM theory can be found in our previous paper mentioned above. Briefly, electrons in an atomic system can be divided into the weakest bound electron (WBE) and the nonweakest bound electrons (NWBEs) from the angle of dynamic ionization, in which the electrons are supposed to be excited or ionized one by one. The electron which most weakly bound to the system, and thus apt to be excited or ionized first, is called the WBE and the others NWBEs. Furthermore, the WBE is supposed to move in the central potential field due to the ion core formed by NWBEs and the nucleus. The problem of a multi-electron system can therefore be simplified to a problem of a single-electron of WBE, for WBEi the Schrödinger equation is:

$$\left[-\frac{1}{2}{\nabla_i}^2 + V(r_i)\right]\psi_i = \varepsilon_i\psi_i \tag{1}$$

in which the potential exerted on the WBE is suggested to be:

$$V(r_i) = -\frac{Z'}{r_i} + \frac{d(d+l)+2dl}{2{r_i}^2} \qquad \text{(in a.u.)} \tag{2}$$

Substituting Eq.(2) into Eq.(1), and solving the above Schrödinger equation of WBE, we obtain the expression of energy eigenvalue and the radial function R of the WBE:

$$\varepsilon_i = -\frac{Z'^2}{2n'^2} \tag{3}$$

$$R(r) = A\exp\left(-\frac{Z'r}{n'}\right) r^{l'} L^{2l'+1}_{n-l-1}\left(\frac{2Z'r}{n'}\right) \tag{4}$$

where Z' is the effective (not net) nuclear charge number, n' is the effective principal quantum number with n'=n+d, and l' is the effective azimuthal quantum number with l'=l+d .

It is clear that in order to obtain the energy of the WBE the parameters Z' and d must be known. At present, however, we have not found a way to determine those values theoretically. For this reason, a coupled equation is derived for parameter determination by use of the experimental energy levels and the expectation value of the radial distance. The relationship between the energy ε in Eq.(3) and the spectral energy level of the WBE is:

$$E_{\text{spec}} \approx -\varepsilon = \frac{Z'^2}{2n'^2} \tag{5}$$

where E_{spec} can be readily obtained from the experimental energy level T_{spec} and the ionization limit T_{lim} as :

$$E_{\text{spec}} = T_{\text{lim}} - T_{\text{spec}} \tag{6}$$

By use of radical wave function R of the WBE, the matrix element $\langle n_f l_f\,|r|\,n_i l_i\rangle$ relating to the transition from the level (n_f, l_f) to the level (n_i, l_i) can be determined [35] and further the radial expectation value $\langle r\rangle$ of the WBE:

$$\langle r\rangle = \frac{3n'^2 - l'(l'+1)}{2Z'} \tag{7}$$

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TABLE I The transition probabilities between triplet states

Transition	λ/Å	f	$A/10^8 s^{-1}$	Other transition probabilities			
				Ref.[46]	Ref.[45]	Ref.[29][a]	Ref.[44][b]
3s4s $^3S_1$-3s 4p $^3P^0_0$	4576.039	0.13832	1.322024	1.2371	1.24	1.23	1.25
3s 4s $^3S_1$-3s 4p $^3P^0_1$	4569.121	0.41553	1.327802	1.2414	1.24	1.23	1.25
3s 4s $^3S_1$-3s 4p $^3P^0_2$	4553.898	0.69458	1.340626	1.2571	1.26	1.24	1.26
3s 5s $^3S_1$-3s 4p $^3P^0_0$	3231.428	0.19639	0.418223				0.45
3s 5s $^3S_1$-3s 4p $^3P^0_1$	3234.887	0.19685	1.254919				1.3
3s 5s $^3S_1$-3s 4p $^3P^0_2$	3242.561	0.19787	2.092398				2.3
3s 6s $^3S_1$-3s 4p $^3P^0_0$	1838.466	0.030863	0.203051				0.18
3s 6s $^3S_1$-3s 4p $^3P^0_1$	1839.585	0.030898	0.60911				0.55
3s 6s $^3S_1$-3s 4p $^3P^0_2$	1842.064	0.030976	1.015				0.93
3s 6s $^3S_1$-3s 5p $^3P^0_0$	6836.331	0.29273	0.139284				0.15
3s 6s $^3S_1$-3s 5p $^3P^0_1$	6835.952	0.29270	0.41785				0.44
3s 6s $^3S_1$-3s 5p $^3P^0_2$	6833.439	0.29247	0.696388				0.74
3s 7s $^3S_1$-3s 5p $^3P^0_0$	3683.290	0.044691	0.073253				0.067
3s 7s $^3S_1$-3s 5p $^3P^0_1$	3683.180	0.044689	0.219762				0.20
3s 7s $^3S_1$-3s 5p $^3P^0_2$	3682.451	0.044676	0.366308				0.33
3s 4p $^3P^0_0$-3s 3d $^3D_1$	3097.725	0.088115	1.837734	1.6947	1.86	1.72	
3s 4p $^3P^0_0$-3s 4d $^3D_1$	3792.516	1.1833	1.829462	1.7956	1.73		2.0
3s 4p $^3P^0_1$-3s 3d $^3D_1$	3094.553	0.066049	0.460117	0.42402	0.465	0.430	
3s 4p $^3P^0_1$-3s 3d $^3D_2$	3094.322	0.11888	1.380494	1.2722	1.40	1.29	
3s 4p $^3P^0_1$-3s 4d $^3D_1$	3797.281	0.29585	1.368733	1.3394	1.29		1.5
3s 4p $^3P^0_1$-3s 4d $^3D_2$	3797.202	0.88754	2.463833	2.4128	2.32		2.6
3s 4p $^3P^0_2$-3s 3d $^3D_1$	3087.562	0.004398	0.018465	0.017062	0.0187	0.0173	
3s 4p $^3P^0_2$-3s 3d $^3D_2$	3087.333	0.039578	0.277001	0.25610	0.281	0.259	
3s 4p $^3P^0_2$-3s 3d $^3D_3$	3087.132	0.15830	1.551347	1.4334	1.57	1.45	
3s 4p $^3P^0_2$-3s 4d $^3D_1$	3807.860	0.011835	0.090753	0.088795	0.0855		0.095
3s 4p $^3P^0_2$-3s 4d $^3D_2$	3807.780	0.17753	0.816816	0.79989	0.770		0.88
3s 4p $^3P^0_2$-3s 4d $^3D_3$	3807.606	0.99417	3.2676	3.2021	3.08		3.4
3s 5p $^3P^0_0$-3s 4d $^3D_1$	7463.951	0.18549	0.66634				0.63
3s 5p $^3P^0_0$-3s 5d $^3D_1$	8274.221	1.5131	0.49145				0.51
3s 5p $^3P^0_1$-3s 4d $^3D_1$	7464.402	0.13912	0.16657				0.16
3s 5p $^3P^0_1$-3s 4d $^3D_2$	7464.709	0.25042	0.49968				0.49
3s 5p $^3P^0_2$-3s 4d $^3D_1$	7467.401	0.009276	0.006658				0.0065
3s 5p $^3P^0_2$-3s 4d $^3D_2$	7467.708	0.083485	0.099869				0.097
3s 5p $^3P^0_2$-3s 4d $^3D_3$	7468.378	0.33395	0.55919				0.54
3s 5p $^3P^0_2$-3s 5d $^3D_1$	8269.985	0.01513	0.024596				0.026
3s 5p $^3P^0_2$-3s 5d $^3D_2$	8267.920	0.226950	0.22148				0.23
3s 5p $^3P^0_2$-3s 5d $^3D_3$	8264.838	1.2709	0.88656				0.91
3s 6p $^3P^0_0$-3s 4d $^3D_1$	3047.170	0.010269	0.22135				0.22
3s 6p $^3P^0_1$-3s 4d $^3D_1$	3045.932	0.007732	0.055594				0.055
3s 6p $^3P^0_1$-3s 4d $^3D_2$	3045.983	0.013916	0.16677				0.17
3s 6p $^3P^0_2$-3s 4d $^3D_1$	3044.654	0.000517	0.002234				0.0023
3s 6p $^3P^0_2$-3s 4d $^3D_2$	3044.705	0.004657	0.033513				0.033
3s 6p $^3P^0_2$-3s 4d $^3D_3$	3044.817	0.018626	0.18764				0.19
3s 7p $^3P^0_0$-3s 5d $^3D_1$	5603.016	0.015850	0.10104				0.10
3s 7p $^3P^0_1$-3s 5d $^3D_1$	5601.560	0.011916	0.025335				0.025
3s 7p $^3P^0_1$-3s 5d $^3D_2$	5602.508	0.021434	0.075924				0.077
3s 7p $^3P^0_2$-3s 5d $^3D_1$	5598.440	0.000798	0.001020				0.0010

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Table I Continued

Transition	λ/Å	f	$A/10^8 s^{-1}$	Other transition probabilities from Ref			
				Ref.[46]	Ref.[45]	Ref.[29][a]	Ref.[44][b]
3s 7p $^3P^0_2$-3s 5d $^3D_2$	5599.386	0.007181	0.015279				0.015
3s 7p $^3P^0_2$-3s 5d $^3D_3$	5600.801	0.028693	0.085429				0.086
3s 4d $^3D_1$-3s 5f $^3F^0_2$	3487.970	0.44055	1.4494				1.5
3s 4d $^3D_1$-3s 6f $^3F^0_2$	2450.191	0.15207	1.0139				1.0
3s 4d $^3D_2$-3s 5f $^3F^0_2$	3488.037	0.048954	0.26843				0.28
3s 4d $^3D_2$-3s 5f $^3F^0_3$	3487.925	0.39153	1.5336				1.6
3s 4d $^3D_2$-3s 6f $^3F^0_2$	2450.224	0.016897	0.18776				0.19
3s 4d ^{3}D3-3s 6f $^3F^0_4$	2450.247	0.13965	1.2070				1.2
3s 5d $^3D_1$-3s 4f $^3F^0_2$	5698.074	0.060729	0.20796				0.20
3s 5d $^3D_1$-3s 6f $^3F^0_2$	6523.289	0.32716	0.30774				0.32
3s 5d $^3D_2$-3s 4f $^3F^0_2$	5697.094	0.011237	0.023096				0.022
3s 5d $^3D_2$-3s 4f $^3F^0_3$	5706.173	0.064542	0.18513				0.18
3s 5d $^3D_2$-3s 6f $^3F^0_2$	6524.574	0.036394	0.057033				0.060
3s 5d $^3D_2$-3s 6f $^3F^0_3$	6524.408	0.29107	0.32583				0.34
3s 5d $^3D_3$-3s 4f $^3F^0_2$	5695.630	0.000321	0.000471				0.00045
3s 5d $^3D_3$-3s 4f $^3F^0_3$	5704.705	0.008058	0.016517				0.016
3s 5d $^3D_3$-3s 4f $^3F^0_4$	5717.873	0.07306	0.19167				0.19
3s 5d $^3D_3$-3s 6f $^3F^0_2$	6526.495	0.000744	0.001631				0.0018
3s 5d $^3D_3$-3s 6f $^3F^0_3$	6526.329	0.026035	0.040777				0.043
3s 5d $^3D_3$-3s 6f $^3F^0_4$	6526.146	0.301164	0.366896				0.39

[a] Calculated from the oscillator strength given in Ref.[29].
[b] Critical data from the NIST.

TABLE II The transition probabilities between singlet states

Transition	λ/Å	f	$A/10^8 s^{-1}$	Other transition probabilities from Ref			
				Ref.[46]	Ref.[45]	Ref.[29][a]	Ref.[44][b]
3s 4s $^1S_0$-3s 4p $^1P^0_1$	5741.326	1.102786	0.74395	0.560	0.524	0.544	0.47
3s 5s $^1S_0$-3s 4p $^1P^0_1$	3186.043	0.176337	3.476636				3.8
3s 6s $^1S_0$-3s 4p $^1P^0_1$	1856.070	0.029664	1.723304				1.6
3s 6s $^1S_0$-3s 5p $^1P^0_1$	6316.206	0.22813	1.144433				1.2
3s 7s $^1S_0$-3s 5p $^1P^0_1$	3570.691	0.03998	0.62756				0.58
3s 4p $^1P^0_1$-3s 3d $^1D_2$	9326.453	0.140353	0.179405	0.082	0.108	0.0540	
3s 4p $^1P^0_1$-3s 4d $^1D_2$	3591.490	1.19715	3.714915	3.256	2.93		3.9
3s 5p $^1P^0_1$-3s 4d $^1D_2$	9802.595	0.348947	0.403761				0.39
3s 5p $^1P^0_1$-3s 5d $^1D_2$	7614.453	1.488105	1.02732				1.1
3s 7p $^1P^0_1$-3s 5d $^1D_2$	5811.798	0.023287	0.076654				0.078
3s 3d $^1D_2$-3s 4f $^1F^0_3$	2559.963	1.067134	7.759286	1.802	1.59		7.7
3s 4d $^1D_2$-3s 4f $^1F^0_3$	201097.995	0.022543	2.656286×10^{-5}	1.344×10^{-5}	2.03×10^{-5}		
3s 4d $^1D_2$-3s 5f $^1F^0_3$	4717.974	1.130951	2.421046				2.8
3s 4d $^1D_2$-3s 6f $^1F^0_3$	2529.231	0.139392	1.038316				0.81
3s 5d $^1D_2$-3s 4f $^1F^0_3$	4378.853	0.017704	0.086235				0.085
3s 5d $^1D_2$-3s 6f $^1F^0_3$	6171.540	0.102809	0.128621				0.12

[a] Calculated from the oscillator strength given in Ref.[29].
[b] Critical data from the NIST.

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Thus a coupled equation comprising Eq.(5) and Eq.(7) is derived:

$$\begin{cases} E_{\rm spec} = \dfrac{Z'^2}{2n'^2} \\ \langle r\rangle = \dfrac{3n'^2 - l'(l'+1)}{2Z'} \end{cases} \quad (8)$$

here the values of E_{spec} can be obtain from experimental data, and $\langle r\rangle$ can be evaluated by various theoretical methods such as numerical Coulomb approximation (NCA), RHF, MCHF, Hartree-Slater(HS), HKS, TDHF, and self-interaction-corrected local spin density (SIC-LSD)[36-42]. With the parameters Z', l' and n', the transition probabilities of (n_f, l_f) to (n_i, l_i) for spontaneous emission *($E_f > E_i$)* can be calculated:

$$\begin{aligned} A_{fi} &= 2.027\times10^{-14}(E_f-E_i)^3\,|\langle n_f l_f\,|r|\,n_i l_i\rangle|^2 \\ &\quad\times(2L_f+1)(2L_i+1)\,(2J_i+1)\,l_\rangle W^2 \\ &\quad\times(l_i L_i l_f L_f; L_c 1) W^2(L_i J_i L_f J_f; S1)\,\text{(in a.u.)} \end{aligned} \quad (9)$$

in which $l_\rangle = \max(l_f, l_i)$, E_f and E_i are the spectral energy levels of f and i, L_c is the total orbital angular momentum of the atomic core, and *W(abcd;ef)* the Racah coefficient [43].

III. RESULTS

The spin-allowed transition probabilities between energy levels above the 3s3p of Si III were calculated within the WBEPM theory. In the parameter determinations, energy levels were taken from Ref.[44] and the radial expectation values $\langle r\rangle$ were evaluated from the numerical coulomb approximation (NCA). The results for transitions probabilities together with wavelength λ and oscillator strength f for triplet states were shown in Table I and those for singlet states in Table II. Comparisons of the results with the critical data from the NIST [44], values from a calculation based on a multiconfiguration approach [45], data from an MCHF calculation [46] and results from an MCOPM calculation [29] are also made.

It can be seen that most of our results agree well with those from the NIST, with the discrepancy less than 15%. For the critically evaluated NIST data listed in Table I, except for 4s ^{3}S-4p ^{3}P^0 transitions for which the uncertainties are less than 25%, the others have an uncertainty of about 50%, or more. For transitions for which there is no comparable data available in the NIST, e.g. 4p ^{3}P^0 - 3d ^{3}D transitions, our results are much closer to those from Ref.[45] in which the results of some cases are very close to the data from the NIST. Fischer *et al.* has performed an MCHF calculation for transitions between several low-lying excited states and obtained satisfactory results for most cases [46]. In Ref.[29], Aashamar *et al.* calculated the oscillator strength for downward transitions in Si III from 3s4s and 3s4p levels using MCOPM with inclusion of relativistic corrections, and the results showed a good L-V agreement for oscillator strengths. We transform the values of oscillator strengths given in Ref.[29] into transition rates in order to make a comparison with our transition rates values.

Table II gives the results for transitions between singlet states, and shows comparisons with others' results. From the comparison we can see that except for the 4s ^{1}S$_0$-4p ^{1}P$_1^0$ transition for which the discrepancy exceeds 50%, the results show a high agreement with the critical data. And for transitions unavailable from the NIST, namely 4p ^{1}P$_1^0$-3d ^{1}D$_2$ and 4d ^{1}D$_2$-4f ^{1}F$_3^0$ transitions, the results are close to those from Ref.[45], which is consistent with the cases for triplet states. Note that in contrast to the good agreement between the results for triplet states, those from the currently available sources for singlet states bear a large discrepancy as can be seen from the 4p ^{1}P$_1^0$-3d ^{1}D$_2$ transition in Table II. For this transition the result given by Nussbaumer [45] is one-half the one from Aashamar. Another case is the 4d ^{1}D$_2$-4f ^{1}F$_3^0$ transition as listed in column A and B of Table I. Table III compares our results with those obtained from others methods for multiplet strengths.

As a whole, our results show a better agreement with the critical data than the others do. Another important fact clearly shown in Tables I and II is that there exist many gaps in other work for transitions involving states with $n\geq5$ where our results account well with the critical data and data in the NIST for certain transitions. The gaps are thought to be due to the theoretical difficulties as noted earlier in the introduction.

It is noted that in the coupled equation derived within the WBEPM theory to determine the parameters needed in the transition probabilities evaluation, $\langle r\rangle$ is evaluated by the method of NCA. NCA has been proved to be an economical approximation which gives results for excited states, especially highly excited states, that account well with those from other methods [39,47]. When it comes to lower states, however, the method will result in larger differences. Resonance transitions in atomic carbon and oxygen were investigated[48]. There the RHF method was used to evaluate the $\langle r\rangle$ for the ground states, and reasonable accuracy was achieved. Since the value of $\langle r\rangle$ is directly related to the accuracy of the results, it is believed that more accurate $\langle r\rangle$ will improve the agreement between the calculated results and the experimental ones.

IV. CONCLUSION

The spin-allowed transition probabilities were calculated between energy levels above the 3s3p state of Si III with a satisfactory accuracy. The good agreement with the critical data proves that WBEPM theory is reliable. Furthermore, the computational method is simple and can readily be applied to transition calculations for

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TABLE III Multiplet oscillator strengths

Transition	This work	Exp.[14]	Theory				
			Ref.[29]	Ref.[49]	Ref.[45]	Ref.[33]	Ref.[5]
3s 4s ^{3}S-3s 4p ^{3}P^0	1.248	0.92	1.16	1.17[a], 1.173[b], 1.24[c]	1.153	1.16	1.1715
3s 4s ^{3}S-3s 5p ^{3}P^0	0.004879			0.0087[a], 0.0063[b], 0.0027[c]		0.0143	
3s 5s ^{3}S-3s 4p ^{3}P^0	0.1973			0.24[a], 0.23[b], 0.21[c]		0.232	
3s 5s ^{3}S-3s 5p ^{3}P^0	1.604					1.49	
3s 6s ^{3}S-3s 4p ^{3}P^0	0.03094			0.032[a], 0.0300[b], 0.030[c]		0.0357	
3s 6s ^{3}S-3s 5p ^{3}P^0	0.2926			0.33[a], 0.21[b], 0.31[c]		0.328	
3s 7s ^{3}S-3s 3p ^{3}P^0	0.002236					0.0044	
3s 7s ^{3}S-3s 4p ^{3}P^0	0.01159			0.013[a], 0.010[c]		0.0172	
3s 7s ^{3}S-3s 5p ^{3}P^0	0.04468			0.039[a], 0.041[c]		0.0445	
3s 4p ^{3}P^0-3s 3d ^{3}D	0.1584	0.12	0.154	0.137[a], 0.156[b], 0.133[c]	0.1535	0.159	0.1427
3s 4p ^{3}P^0-3s 4d ^{3}D	1.183	0.80		1.21[a], 1.12[b], 1.14[c]	1.13333	1.11	
3s 4p ^{3}P^0-3s 5d ^{3}D	0.03403			0.0056[a], 0.0068[b], 0.012[c]		0.0070	
3s 5p ^{3}P^0-3s 3d ^{3}D	0.008399			0.00021[a], 0.0254[b]		0.00002	
3s 5p ^{3}P^0 − 3*s*4*d*^{3}D	0.3339					0.326	
3s 5p ^{3}P^0-3s 5d ^{3}D	1.513			1.57[a], 1.61[b]		1.45	
3s 5p ^{3}P^0-3s 6d ^{3}D	0.03900			0.038[a], 0.0478[b]		0.0290	
3s 6p ^{3}P^0-3s 3d ^{3}D	0.002836			0.0058[a], 0.0068[b], 0.0148[c]			
3s 3d ^{3}D-3s 4f ^{3}F^0	0.7126	0.42		0.987[a]			
3s 3d ^{3}D-3s 5f ^{3}F^0	0.1915			0.27[a], 0.194[c]			
3s 3d ^{3}D-3s 6f ^{3}F^0	0.07877			0.104[a], 0.082[c]			
3s 3d ^{3}D-3s 7f ^{3}F^0	0.04095			0.043[a], 0.043[c]			
3s 4d ^{3}D-3s 4f ^{3}F^0	0.4713			0.349[a]			
3s 4d ^{3}D-3s 5f ^{3}F^0	0.4404	0.27		0.391[a], 0.449[c]			
3s 4d ^{3}D-3s 6f ^{3}F^0	0.1521			0.136[a], 0.152[c]			
3s 5d ^{3}D-3s 4f ^{3}F^0	0.07272			0.0900[a]			
3s 6d ^{3}D-3s 4f ^{3}F^0	0.008770			0.027[a]			
3s 4s ^{1}S-3s 4p ^{1}P^0	1.103		0.807	0.056[a], 0.740[b]	0.766	0.741	0.7429
3s 4s ^{1}S-3s 5p ^{1}P^0	0.05448			0.0081[a], 0.307[b]		0.192	
3s 5s ^{1}S-3s 4p ^{1}P^0	0.1763			0.21[a], 0.205[b], 0.193[c]		0.199	
3s 5s ^{1}S-3s 5p ^{1}P^0	1.309					1.17	
3s6s ^{1}S-3s 4p ^{1}P^0	0.02966			0.043[a], 0.0403[b], 0.028[c]			
3s 7s ^{1}S-3s 4p ^{1}P^0	0.01129			0.021[a], 0.01[b]			
3s 4p ^{1}P^0-3s 3d ^{1}D	0.1404	0.060		0.096[a], 0.0958[b]	0.0618	0.0806	0.0597
3s 4p ^{1}P^0-3s 4d ^{1}D	1.197	0.45	0.984	0.937[a], 0.933[b], 1.22[c]		0.949	
3s 4p ^{1}P^0-3s 5d ^{1}D	0.04019			0.008[a], 0.012[b], 0.033[c]		0.0143	
3s 5p ^{1}P^0-3s 3d ^{1}D	0.001404			0.058[a], 0.017[b]		0.0125	
3s 5p ^{1}P^0-3s 4d ^{1}D	0.3489			0.25[a], 0.284[b]		0.301	
3s 5p ^{1}P^0-3s 5d ^{1}D	1.488					1.31	
3s 6p ^{1}P^0-3s 3d ^{1}D	8.082×10^{-6}			0.052[a], 0.0002[b]			
3s 6p ^{1}P^0-3s 4d ^{1}D	0.01141			0.046[a], 0.071[b]			
3s 3d ^{1}D-3s 4f ^{1}F^0	1.067			0.430[a]	0.2002		
3s 3d ^{1}D-3s 5f ^{1}F^0	0.004960			0.20[a]			
3s 3d ^{1}D-3s 6f ^{1}F^0	0.07076			0.85[a]			
3s 3d ^{1}D-3s 7f ^{1}F^0	0.02545			0.702[a]			
3s 4d ^{1}D-3s 5f ^{1}F^0	1.131			0.672[a], 1.31[c]			
3s 4d ^{1}D-3s 6f ^{1}F^0	0.1394			0.16[a]			
3s 4d ^{1}D-3s 7f ^{1}F^0	0.07624			0.268[a]			

[a] Semiempirical frozen core potential. [b] Modified Hartree-Fock-Slaterbasis set. [c] Coulomb approximation.

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highly states. Considering that in previously published results there are remaining blanks in these transitions and transitions where large discrepancy exists, our work will benefit both experimental studies and theoretical ones. On the other hand, the forbidden transitions, for example, singlet-triplet, are still impossible to study by this method.

As mentioned above, we have calculated transition probabilities for several Mg-like ions in our previous work. In order to see how regulation of results changed with charge number of the nucleus, we give the following figures. Figure 1 shows different transitions, 3s 4p $^3P_0^0$-3s 4d $^3D_1$, 3s 4p $^3P_1^0$-3s 4d $^3D_1$, and 3s 4p $^3P_2^0$-3s 4d $^3D_1$, for which the only difference between those transitions is the J value of initial state 3s4p. We can see that as the charge number Z become bigger the transition probabilities become higher and as the J value of state 3s 4p$^3P_0^0$ changes from 0 to 2 the amplitude of the curve reduced. In Fig.2, the principal numbers are the same: 3s3p-3s3d and 3s4p-3s4d, also as the charge number Z become bigger the transition probabilities become higher and as the principal numbers changes from 3 to 4 the amplitude of the curve reduced. From Fig.3, we can see the relative deviation of our calculations is almost the same between the transitions whose only difference is the J value of initial state of the same ion, and as the charge number Z become bigger the results become more accurate.

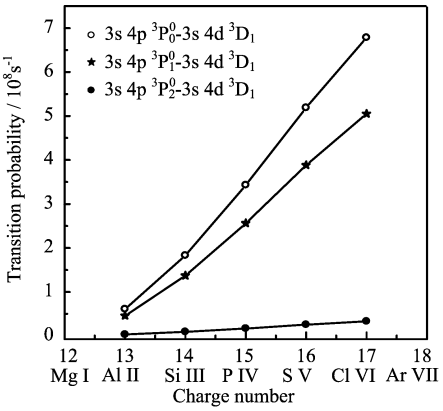

FIG. 1 Charge number Z *vs.* transition rates T for transitions between initial 3s 4p ($^3P_0^0$, $^3P_1^0$, $^3P_2^0$) and 3s 4d $^3D_1$.

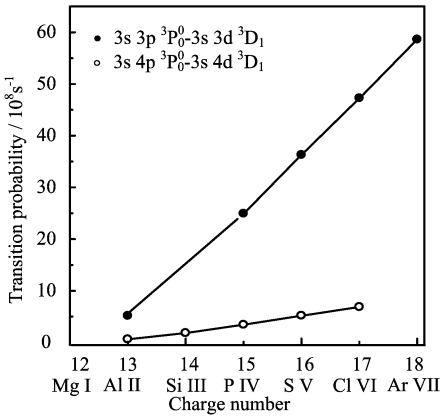

FIG. 2 Charge number Z *vs.* transition rates T for transitions 3s 3p $^3P_0^0$ - 3s 3d $^3D_1$ and 3s 4p $^3P_0^0$ - 3s 4d $^3D_1$.

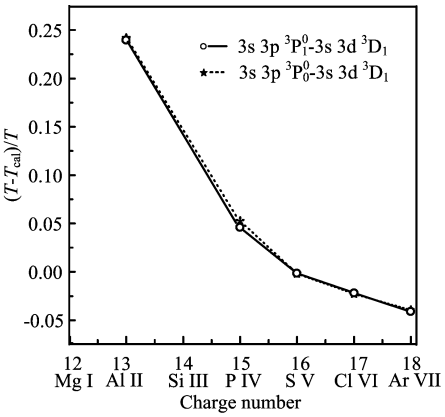

FIG. 3 Charge number Z *vs.* $(T\text{-}T\mathrm{cal})/T$ for transitions 3s 3p $^3P_0^0$-3s 3d $^3D_1$ and 3s 3p $^3P_0^0$-3s 3d $^3D_1$.

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