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Doubly excited triplet states of highly stripped ions

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Abstract. Transition energies, Coulomb repulsions and effective quantum numbers have been calculated for the doubly excited $Nsnp$: $^3P^0$ (for $N = 2$, $n = N, \ldots, 5$); $Nsnd$: $^3D^e$ (for $N = 2$, $n = N+1, \ldots, 5$) and $Npnd$: $^3F^0$ (for $N = 2$, $n = N+1, \ldots, 5$) states for the highly stripped ions Na^{9+}, Mg^{10+}, Al^{11+}, Si^{12+}, P^{13+} and S^{14+}. Time-dependent perturbation theory has been applied to calculate such transitions properties. A time-dependent harmonic perturbation causes simultaneous excitation of both the electrons with a change of spin state. The doubly excited energy levels and the analytic representation of their wave functions are obtained by identifying the poles of an appropriately constructed linearized variational functional with respect to driving frequency. Most of the results are new. The transition energies and effective quantum numbers of $2s2p$: $^3P^0$ states of all the ions agree well with the only available experimental data.

PACS. 31.50.+w Excited states – 32.80.Dz Autoionization

1 Introduction

Doubly excited states play an important role in a wide range of atomic and molecular processes. The dynamics and spectroscopy of the doubly excited states are the subject of current interest because the understanding of these states requires a fundamental departure from the conventional independent particle model and a new set of quantum numbers is necessary to designate such levels [1,2]. These states are very useful for diagnostic of laboratory and astrophysical plasmas and also play a major role in multielectron phenomena in ion atom collisions and particularly in dielectronic recombination processes which occur in low-density coronal plasma where the distribution of atoms among various ionization stages and in turn the coronal equilibrium is mainly guided by the balance between the rates of various detailed ionization and recombination processes; one is the inverse of the other [3,4]. He-like ions are often prominent in high-temperature plasma occurring in astrophysics and in the laboratory. SXV is an ion suitable to diagnose plasmas of a temperature at about 10^7 K, because it has the maximum fractional abundance around there. The Bragg crystal spectrometer carried by the YOHKOH satellite detects soft X-rays from SXV in the solar corona to provide information on the coronal plasma [5,6]. Moreover, NaX, MgXI, AlXII, SiXIII, PXIV and SXV are detected spectroscopically in plasmas of the upper solar atmosphere [7] and also by observing coronal lines due to the decay of doubly excited states in such ions [8].

After the pioneering photoabsorption measurements of Madden and Codling [9,10] on helium, a number of theoretical [11–14] and experimental [15–18] approaches so far adopted to study the doubly excited states but their investigations are confined to He and in some cases to the few members of the He isoelectronic sequence. The experimental results are now available for the doubly excited states of highly stripped ions [19–24]. It should be mentioned here that no theoretical results so far reported in the literature on these systems. Very recently we have developed and applied a method [25,26] based on time-dependent variation perturbation theory (TDVPT) to study the doubly excited triplet states of two-electron atomic systems. The theory has achieved a fair amount of success in predicting the transition energies of the doubly excited triplet states of the first four members of the He isoelectronic sequence. In this method a spin-dependent harmonic perturbation is applied on the system. The perturbation operator is such that it alters the spatial symmetry of both the orbitals simultaneously and changes the spin symmetry from singlet to triplet. The description of the perturbed wave function is essentially correlated. A linearized variational functional is constructed along the same line as has been discussed by [27,28]. The response of the electronic charge cloud towards such a perturbation is studied by varying the external frequency. The functional has poles at certain frequencies which furnish the transition energies to the doubly excited states. From a study of the behavior of the perturbed function at the singularities, analytic representations of the doubly excited functions can be obtained which are utilized for studying such transition properties.

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In this communication we report the calculations for a few low and moderately high lying doubly excited $^3P^0$, $^3D^e$, and $^3F^0$ states of Na^{9+}, Mg^{10+}, Al^{11+}, Si^{12+}, P^{13+} and S^{14+} from their ground state $^1S^e$. A brief review of the theory is discussed in Section 2, followed by discussions of theoretical results in Section 3.

2 Theory

The two-electron ions are described by the usual non-relativistic Hamiltonian H_0 (we use a.u. throughout) and a spin-dependent harmonic perturbation of the form

$$H'(\bar{r},\bar{\sigma},t) = G(\bar{r},\bar{\sigma})e^{-i\omega t} + G^{+}(\bar{r},\bar{\sigma})e^{i\omega t} \tag{1}$$

is applied on the system, where the perturbation $G(\bar{r},\bar{\sigma})$ is such that it excites both the electrons simultaneously to a new state changing the spin multiplicity from singlet to triplet. A suitable choice of the perturbation may be

$$\begin{aligned} G(\bar{r},\bar{\sigma}) = \lambda[h(\bar{r}_1)h'(\bar{r}_2) - h(\bar{r}_2)h'(\bar{r}_1)] \\ \times[S_-(1)S_+(2) - S_-(2)S_+(1)]\,, \end{aligned} \tag{2}$$

where λ is the perturbation strength parameter, S_+ and S_- are the usual spin-up and spin-down operators. The spatial term excites both the electrons from the ground state. The general structure of the one-particle term is given by

$$h(\bar{r}) \approx r^l P_l(\cos\vartheta)\,, \tag{3}$$

where $l = 0, 1, 2, \ldots$, will excite the ground-state s orbital to s, p, $d, \ldots$, symmetries, respectively. Under the action of this perturbation the time evolution of the total wave function may be written as

$$\Phi(\bar{r},t) = N[\Psi(\bar{r}) + \delta\Psi^-(\bar{r})e^{-i\omega t} + \delta\Psi^+(\bar{r})e^{i\omega t}]e^{iE_0 t}, \tag{4}$$

where $\delta\Psi^{\pm}$ are the first-order admixtures to the ground-state function Ψ due to two components of the harmonic perturbation and E_0 is the ground-state energy. The normalization constant N is determined from the condition

$$\frac{1}{T}\int_0^T \langle\Phi|\Phi\rangle \mathrm{d}t = 1\,. \tag{5}$$

Since the perturbation (Eq. (2)) changes the spin multiplicity, the spin part of Ψ and $\delta\Psi^{\pm}$ are different. To determine the time evolution of the total wave function we have to determine the first-order perturbed functions $\delta\Psi^{\pm}$. These are obtained by constructing a time-averaged (time averaging is performed over the time period T of the harmonic perturbation) functional

$$J(\Phi) = \frac{1}{T}\int_0^T \langle\Phi|H_0 + H' - i\partial/\partial t|\Phi\rangle \mathrm{d}t\,, \tag{6}$$

subject to the optimization condition

$$\delta J(\Phi) = 0\,. \tag{7}$$

The optimization is done with respect to the variation parameters introduced in $\delta\Psi^{\pm}$. We expand the spatial part of $\delta\Psi^{\pm}$ in the following way:

$$\delta\Psi^{\pm} = \sum_i C_i^{\pm}\eta_i(1,2)\,, \tag{8}$$

where $\eta_i(1,2)$ are correlated pair bases formed out of suitable one-particle Slater orbital (STOs) products [25]

$$\eta_i(1,2) \approx \xi_k(1)\xi_l'(2) - \xi_k(2)\xi_l'(1) \tag{9}$$

and $C_i^{\pm}$ are the linear variation parameters. The choice of the exponents of the Slater bases depends on the symmetry and the principal quantum number of the excited orbitals and are preassigned here. We expand the functional (Eq. (6)) in terms of $\delta\Psi^{\pm}$ and retain terms up to quadratic in $\delta\Psi^{\pm}$. The optimization condition

$$\frac{\partial J(\Phi)}{\partial C^{\pm}} = 0 \tag{10}$$

leads to sets of decoupled linear equations in the unknow parameters $C^{\pm}$ [25] which can readily be solved for a given external frequency to get the response characteristics of the systems. The present calculation is non-relativistic. Breit and other relativistic corrections can be ignored at the present level of accuracy. A discussion of the results is given in the next section.

3 Results and discussions

In this present communication, we have calculated transition energies, Coulomb repulsion and effective quantum numbers of the doubly excited triplet transitions *viz.* $1s^2$: $^1S^e \rightarrow Nsnp$: $^3P^0(N = 2,\ n = N, \ldots, 5)$; *Nsnd*: $^3D^e(N = 2,\ n = N+1, \ldots, 5)$ and *Npnd*: $^3F^0(N = 2,\ n = N+1, \ldots, 5)$ for the highly stripped ions Na^{9+}, Mg^{10+}, Al^{11+}, Si^{12+}, P^{13+} and S^{14+}. We have used improved Roothaan-Hartree-Fock (RHF) ground-state functions of Koga *et al.* [29] for all ions under present consideration. For all the perturbed functions, 9 parameter STO representation has been used for the excited orbitals, the exponents being preassigned. The choice of the exponents depends on the symmetry and principal quantum number of the orbitals concerned. Since we are considering excitations of different orbital symmetry, we get 81 linear variation parameters of the product bases from nine parameter description of the orbitals. The parameters are determined through optimization and furnish a very reasonable description of the perturbed wave function at each frequency. The optimized functional $J(\Phi)$ increases continuously and regularly with respect to the driving frequency ω with real poles at certain frequency. The pole positions determine the doubly excited modes of the unperturbed Hamiltonian and hence the positions of these poles furnish the doubly excited energy levels measured from the ground state of the systems. The first-order perturbed function $\delta\Psi^-$ blows up at pole positions and the

Table 1. Energies (measured from ground state), Coulomb repulsions and effective quantum numbers (n^*) of the doubly excited $^3P^0$ states of the highly stripped ions below the $N = 2$ hydrogenic threshold.

Ions	States	$N(K,T)_n^A$	Energies (a.u.)			Coulomb repulsions (a.u.)	Effective quantum numbers	
			Theory[α]	Theory[β]	Observed[a]	Theory	Theory	Observed[a]
Na^{9+}	$2s2p$	$2(1,0)_2^+$	85.4379	85.6330	85.5682	1.4177	1.9123	1.9081
	$23sp^+$	$2(1,0)_3^+$	93.2636	93.4587		0.8504	2.9239	
	$23sp^-$	$2(0,1)_3^-$	93.3545	93.5496		0.9389	2.9469	
	$24sp^+$	$2(1,0)_4^+$	95.8687	96.0638		0.5404	3.9269	
	$24sp^-$	$2(0,1)_4^-$	95.9246	96.1197		0.5668	3.9612	
	$25sp^+$	$2(1,0)_5^+$	97.0740	97.2691		0.3388	4.9543	
	$25sp^-$	$2(0,1)_5^-$	97.1044	97.2995		0.3604	4.9916	
Mg^{10+}	$2s2p$	$2(1,0)_2^+$	102.2010	102.4631	102.3702	1.5504	1.9201	1.9147
	$23sp^+$	$2(1,0)_3^+$	111.5671	111.8292		0.9320	2.9307	
	$23sp^-$	$2(0,1)_3^-$	111.6665	111.9286		1.0285	2.9516	
	$24sp^+$	$2(1,0)_4^+$	114.7025	114.9646		0.5607	3.9343	
	$24sp^-$	$2(0,1)_4^-$	114.7616	115.0237		0.6154	3.9644	
	$25sp^+$	$2(1,0)_5^+$	116.1420	116.4041		0.3599	4.9500	
	$25sp^-$	$2(0,1)_5^-$	116.1748	116.4369		0.3921	4.9832	
Al^{11+}	$2s2p$	$2(1,0)_2^+$	120.4647	120.8145	120.6886	1.6827	1.9267	1.9204
	$23sp^+$	$2(1,0)_3^+$	131.5236	131.8734		1.0127	2.9387	
	$23sp^-$	$2(0,1)_3^-$	131.6219	131.9717		1.1181	2.9561	
	$24sp^+$	$2(1,0)_4^+$	135.2271	135.5769		0.6160	3.9417	
	$24sp^-$	$2(0,1)_4^-$	135.2927	135.6425		0.6743	3.9699	
	$25sp^+$	$2(1,0)_5^+$	136.9501	137.2999		0.4236	4.9733	
	$25sp^-$	$2(0,1)_5^-$	136.9866	137.3364		0.4438	5.0048	
Si^{12+}	$2s2p$	$2(1,0)_2^+$	140.2258	140.6840	140.5173	1.8152	1.9321	1.9250
	$23sp^+$	$2(1,0)_3^+$	153.1053	153.5635		1.0950	2.9430	
	$23sp^-$	$2(0,1)_3^-$	153.2097	153.6679		1.2082	2.9589	
	$24sp^+$	$2(1,0)_4^+$	157.4325	157.8907		0.6621	3.9453	
	$24sp^-$	$2(0,1)_4^-$	157.5027	157.9609		0.7279	3.9710	
	$25sp^+$	$2(1,0)_5^+$	159.4386	159.8968		0.4313	4.9689	
	$25sp^-$	$2(0,1)_5^-$	159.4773	159.9355		0.4659	4.9972	
P^{13+}	$2s2p$	$2(1,0)_2^+$	161.4908	162.0895	161.8720	1.9473	1.9370	1.9290
	$23sp^+$	$2(1,0)_3^+$	176.3344	176.9331		1.1788	2.9480	
	$23sp^-$	$2(0,1)_3^-$	176.4460	177.0447		1.2975	2.9627	
	$24sp^+$	$2(1,0)_4^+$	181.3292	181.9279		0.7191	3.9497	
	$24sp^-$	$2(0,1)_4^-$	181.4071	182.0058		0.7835	3.9745	
	$25sp^+$	$2(1,0)_5^+$	183.6457	184.2444		0.5029	4.9713	
	$25sp^-$	$2(0,1)_5^-$	183.7481	184.3468		0.5874	5.0367	
S^{14+}	$2s2p$	$2(1,0)_2^+$	184.2164	184.9919	184.7226	2.0834	1.9399	1.9314
	$23sp^+$	$2(1,0)_3^+$	201.1706	201.9461		1.2569	2.9485	
	$23sp^-$	$2(0,1)_3^-$	201.3012	202.0767		1.3865	2.9635	
	$24sp^+$	$2(1,0)_4^+$	206.9025	207.6780		0.7571	3.9505	
	$24sp^-$	$2(0,1)_4^-$	206.9822	207.7577		0.8312	3.9725	
	$25sp^+$	$2(1,0)_5^+$	209.5766	210.3521		0.5006	4.9809	
	$25sp^-$	$2(0,1)_5^-$	209.6347	210.4102		0.5009	5.0132	

[α] Using RHF ground-state energy [29].

[β] Using experimental ground-state energy [19–24].

[a] Martin *et al.* [19–24].

Table 2. Energies (measured from ground state), Coulomb repulsions and effective quantum numbers (n^*) of the doubly excited $^3D^e$ states of the highly stripped ions below the $N = 2$ hydrogenic threshold.

Ions	States	$N(K,T)_n^A$	Energies (a.u.)		Coulomb repulsions (a.u.)	Effective quantum numbers
			Theory$^\alpha$	Theory$^\beta$	Theory	Theory
Na^{9+}	$2s3d$	$2(0,1)_3^0$	93.4268	93.6219	1.0100	2.9558
	$2s4d$	$2(0,1)_4^0$	95.9377	96.1328	0.5851	3.9694
	$2s5d$	$2(0,1)_5^0$	97.0986	97.2937	0.3843	4.9845
Mg^{10+}	$2s3d$	$2(0,1)_3^0$	111.7467	112.0088	1.1061	2.9688
	$2s4d$	$2(0,1)_4^0$	114.7767	115.0388	0.6414	3.9722
	$2s5d$	$2(0,1)_5^0$	116.1801	116.4422	0.4096	4.9887
Al^{11+}	$2s3d$	$2(0,1)_3^0$	131.7023	132.0521	1.2028	2.9707
	$2s4d$	$2(0,1)_4^0$	135.3006	135.6504	0.6988	3.9734
	$2s5d$	$2(0,1)_5^0$	136.9746	137.3244	0.4535	4.9944
Si^{12+}	$2s3d$	$2(0,1)_3^0$	153.3069	153.7651	1.2991	2.9739
	$2s4d$	$2(0,1)_4^0$	157.5220	157.9802	0.7561	3.9783
	$2s5d$	$2(0,1)_5^0$	159.4759	159.9341	0.4965	4.9962
P^{13+}	$2s3d$	$2(0,1)_3^0$	176.5357	177.1344	1.3953	2.9746
	$2s4d$	$2(0,1)_4^0$	181.4150	182.0137	0.8123	3.9770
	$2s5d$	$2(0,1)_5^0$	183.6845	184.2832	0.5171	4.9958
S^{14+}	$2s3d$	$2(0,1)_3^0$	201.4063	202.1818	1.4918	2.9757
	$2s4d$	$2(0,1)_4^0$	207.0029	207.7784	0.8691	3.9783
	$2s5d$	$2(0,1)_5^0$	209.5900	210.3655	0.5579	4.9883

$^\alpha$Using RHF ground-state energy [29]. $^\beta$Using experimental ground-state energy [19–24].

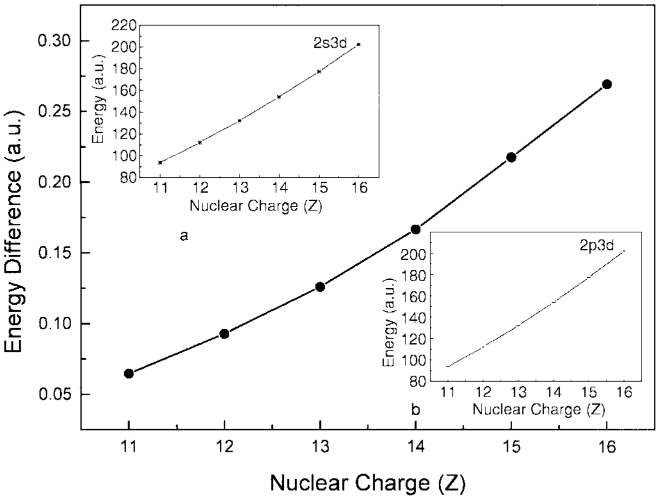

Fig. 1. Plot of the difference of transition energies (a.u.) of $2s2p$: $^3P^0$ states *vs.* nuclear charge (Z) for the highly stripped ions. The insets a and b show, respectively, the plot of the transition energies (a.u.) of $2s3d$: $^3D^e$ and $2p3d$: $^3F^0$ states against Z.

renormalization of the first-order perturbed function at pole position represents adequate description of the doubly excited wave functions. The basic idea of this approach is to scan the eigenspectrum of the unperturbed Hamiltonian adopting a time-dependent viewpoint by probing the system with an external time-dependent stimulus that causes transitions to the doubly excited states of the unperturbed Hamiltonian from the ground state.

The transition energies, Coulomb repulsion integrals and effective quantum numbers of the doubly excited $^3P^0$ states of all the ions obtained by our approach (TDVPT) are displayed in Table 1. The level description has been done according to the configuration scheme of Cooper *et al.* [30]. Such results for the other two doubly excited $^3D^e$ and $^3F^0$ states are listed in Tables 2 and 3, respectively. In all cases transition energies are measured from $^1S^e$ ground sate of the respective ions. The angular part of the two-particle perturbation operator is chosen in such a way that $Nsnp$: $^3P^0$, $Nsnd$: $^3D^e$ and $Npnd$: $^3F^0$ final sates are allowed. The quantum number N, K, T, n and A obtained from group theoretical and hyperspherical coordinate approach [31,32] are also displayed in these tables to have a correspondence with the configuration scheme [33]. In group theoretical and hyperspherical coordinate analysis, effect of radial and angular correlations has been taken care of, whereas our method incorporates radial correlation only.

The only available experimental results [19–24] for the doubly excited $2s2p$: $^3P^0$ states of all the ions are also listed in Table 1 along with our theoretical results for comparison. We have estimated the transition energies both from the RHF ground-state energy of Koga *et al.* [29] and from experimental ground state. These are indicated by the superscript α and β, respectively in Table 1. It is observed from the table that for Na^{9+}, our calculated transition energy is little higher than that of experiment and

Table 3. Energies (measured from ground state), Coulomb repulsions and effective quantum numbers (n^*) of the doubly excited $^3F^0$ states of the highly stripped ions below the $N = 2$ hydrogenic threshold.

Ions	States	$N(K,T)_n^A$	Energies (a.u.)		Coulomb repulsions (a.u.)	Effective quantum numbers
			Theory$^\alpha$	Theory$^\beta$	Theory	Theory
Na^{9+}	$2p3d$	$2(1,0)_3^0$	93.4433	93.6384	1.0255	2.9701
	$2p4d$	$2(1,0)_4^0$	95.9429	96.1380	0.5905	3.9726
	$2p5d$	$2(1,0)_5^0$	97.0970	97.2921	0.3890	4.9825
Mg^{10+}	$2p3d$	$2(1,0)_3^0$	111.7643	112.0264	1.1239	2.9726
	$2p4d$	$2(1,0)_4^0$	114.7823	115.0444	0.6483	3.9751
	$2p5d$	$2(1,0)_5^0$	116.1781	116.4402	0.4263	4.9866
Al^{11+}	$2p3d$	$2(1,0)_3^0$	131.7246	132.0744	1.2223	2.9747
	$2p4d$	$2(1,0)_4^0$	135.3092	135.6590	0.7060	3.9771
	$2p5d$	$2(1,0)_5^0$	136.9732	137.3230	0.4600	4.9932
Si^{12+}	$2p3d$	$2(1,0)_3^0$	153.3233	153.7815	1.3206	2.9765
	$2p4d$	$2(1,0)_4^0$	157.5230	157.9812	0.7637	3.9786
	$2p5d$	$2(1,0)_5^0$	159.4801	159.9383	0.4977	4.9993
P^{13+}	$2p3d$	$2(1,0)_3^0$	176.5608	177.1595	1.4186	2.9780
	$2p4d$	$2(1,0)_4^0$	181.4246	182.0233	0.8209	3.9801
	$2p5d$	$2(1,0)_5^0$	183.6850	184.2837	0.5250	4.9961
S^{14+}	$2p3d$	$2(1,0)_3^0$	201.4347	202.2102	1.5167	2.9791
	$2p4d$	$2(1,0)_4^0$	207.0134	207.7889	0.8786	3.9812
	$2p5d$	$2(1,0)_5^0$	209.5950	210.3705	0.5585	4.9911

$^\alpha$Using RHF ground-state energy [29]. $^\beta$Using experimental ground-state energy [19–24].

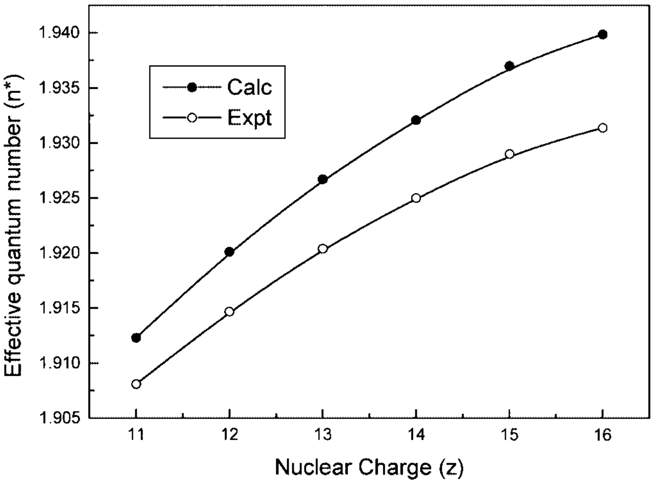

Fig. 2. Plot of effective quantun numbers of $2s2p$: $^3P^0$ states *vs.* nuclear charge (Z) for the highly stripped ions.

the minimum deviation between our calculated transition energy (using experimental ground state) and the experimental value is about 0.07%. The deviation increases as we move towards the higher members and reaches its maximum value of 0.15% for S^{14+}. This discrepancy comes from two sources, namely, the effect of angular correlation and the relativistic effect. The effect of angular correlation decreases as we go over to the higher ionized species because with the increase of nuclear charge (Z), the nuclear potential term dominates over the interelectron Coulomb potential but the relativistic effect increases with the increase of Z. In Figure 1, the difference of transition energy between our calculated values and the experimental results for the $2s2p$: $^3P^0$ states has been plotted against Z. The difference of energy increases as we move towards the higher ionized ions indicating the presence of relativistic effect in such ions. The insets a and b show, respectively, the plot of the transition energies of $2s3d$: $^3D^e$ and $2p3d$: $^3F^0$ states against Z. The smooth behavior of the curves indicates the consistency of our predicted results. Along with the transition energies, we get analytic wave function for the doubly excited states in terms of Slater bases. These analytic wave functions contain a lower number of parameters than those from traditional variational calculation. These wave functions are used to calculate the expectation value of the Coulomb repulsion term in the doubly excited states. The very regular behavior of the expectation values shows the consistency of the excited-state wave functions. These wave functions may be effectively used for collisional calculations involving doubly excited sates, many of which are important in solar chromosphere. As an extra check, we have also calculated the effective quantum numbers (n^*) of the doubly excited energy levels using the formula [14]

$$\varepsilon = -\frac{1}{2}\left[\left(\frac{Z}{N}\right)^2 + \left(\frac{Z-1}{n^*}\right)^2\right], \tag{11}$$

where ε is the energy of the doubly excited energy level (in a.u.) measured from the ionization threshold, N is the principal quantum number of the inner electron and Z is the nuclear charge. It is also observed from the table that our calculated effective quantum number for the $2s2p$: ${}^3P^0$ states of all the ions agree well with the experimental values. It should be specifically mentioned that there are no other theoretical and experimental data so far available in the literature for these states. However, the configuration interaction (CI) calculations could easily be done for the present systems and lead to exact results within the basis set used. The effective quantum numbers (n^*) if the $2s2p$: ${}^3P^0$ states have been plotted against Z in Figure 2 which shows a shift from the experimental one. This shift is due to the fact that any error in calculating the excitation energy makes an appreciable deviation for the value of n^* (Eq. (11)).

Tables 2 and 3 display the transition energies, Coulomb repulsions and effective quantum numbers for the doubly excited $Nsnd$: ${}^3D^e$ and $Npnd$: ${}^3F^0$ states, respectively. There are no theoretical and experimental results available for comparison. However, we can check our calculated transition energies in terms of configuration. The transition energy of $2s3d$: ${}^3D^e$ state will be energetically higher than $2s3p$: ${}^3P^0$ state and the other ${}^3D^e$ states will be higher than the corresponding ${}^3P^0$ states. By similar way, the $2p3d$: ${}^3F^0$ state will be energetically higher than $2s3d$: ${}^3D^e$ state and same for other states also. The transition energies listed in Tables 2 and 3 follow this trend and also the Coulomb repulsion terms are very regular.

In view of the satisfactory agreement with the experimental results for doubly excited $2s2p$: ${}^3P^0$ states and lack of reference data, particularly, for high lying doubly excited ${}^3P^0$, ${}^3D^0$ and ${}^3F^0$ states, our results may serve as a reliable set for future references.

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