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General formalism of the modified atomic orbital theory for the Rydberg series of atoms and ions: application to the photoionization of Ne^+

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Abstract. The general formalism of the Modified orbital atomic theory (MAOT) for the Rydberg series of atoms and ions is presented. Energy resonances of the $2s^22p^4(^1D_2)ns$, nd, $2s^22p^4(^1S_0)ns,nd$ and $2s^2p^5(^3P_2)np$ Rydberg series originating from the $2s^22p^5$ $^2P_{1/2}$ metastable and from the $2s^22p^5$ $^2P_{3/2}$ ground state of Ne^+ are tabulate applying the MAOT formalism. Analysis of the present results is achieved in the framework of the standard quantum defect expansion formula. Comparison is done with the existing experimental and theoretical data.

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Key words: Modified atomic orbital theory (MAOT); Electron correlation calculations for atoms and ions; Rydberg series

1 Introduction

Photoionization of ions is seen to be a fundamental process of importance in many high-temperature plasma environments such as those in stars and nebulae [1] and those in inertial-confinement fusion experiments [2]. Quantitative measurements of photoionization of ions provide precision data on ionic structure, and guidance to the development of theoretical models of multielectron interactions [3]. These measurements are performed mainly using synchrotron radiations such as ASTRID (Aarhus STorage RIng in Denmark) [4], SOLEIL (Source Optimisée de Lumière d'Energie Intermédiaire du LURE (Laboratoire pour l'Utilisation du Rayonnement Electromagntique) in France [5], ALS (Advanced Light Source) in USA [3] and Spring 8 in Japon [6]. The development of these synchrotron light sources has provide high accurate experimental data for benchmarking state-of-the-art theoretical methods of calculations. Among these methods are the

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Hartree-Fock multi-configurationnal (MCDF) method [7, 8], the Quantum Defect Theory [9], the R-matrix approach [10] widely used for international collaborations such as the Opacity Project [11, 12] or the Iron Project [13], the Screening constant by unit nuclear charge (SCUNC) formalism [14, 15]. As far as various ions of great importance for plasma diagnostics are concerned, those of the neon element are one of the prominent candidates due to their frequent use in tokomaks as a diagnostic element for probing plasma [16]. In addition, neon is known to be the sixth most abundant element in the universe and then is of great interest in astrophysics in connection with the role of neon ions in the interpretation of astronomical data from stellar objects such as gaseous nebulas. At ultraviolet wavelengths in the range 300-90 Å, corresponding to a photon energy range of 41 - 138 eV, radiation can photoionize the ground states of several ionization stages of neon such as Ne^{+}, Ne^{2+}, Ne^{3+}, and Ne^{4+}, leaving the residual ion in one of several excited states [3]. These ions and those of carbon (C^{2+}, C^{3+}, C^{4+}), of nitrogen (N^{2+}, N^{3+}, N^{4+}) and of oxygen (O^{2+}, O^{3+}, O^{4+}) are known to contribute to the opacity in the atmospheres of the central stars of planetary nebulas [17, 18]. Using the Advanced Light Source (ALS) devices, Covington *et al.*, [3] presented both high-resolution absolute measurements and theoretical calculations of Ne^{+} at photon energies ranging from the photoionization threshold to 70 eV. These experiments were focused on the $2s^22p^4(^1D_2)ns,nd$, $2s^22p^4(^1S_0)ns,nd$ and $2s^2p^5(^3P_2)np$ Rydberg series originating from both $2s^22p^5\ ^2P_{1/2}$ metastable and $2s^22p^5\ ^2P_{3/2}$ ground state of Ne^{+}. Very recently, Faye *et al.*, [15] used the Screening constant by unit nuclear charge (SCUNC) method to report high lying energy positions of the preceding series. In general, the availability of high-resolution measurements data on ionic species provides great opportunities to verify the accuracy of theoretical predictions or the limitations of a given quantum mechanics model. For this purpose, the General formalism of the Modified orbital atomic theory (MAOT) [19-22] for the Rydberg series of atoms and ions is presented and applied to the photoionization of Ne^{+} considering the same above Rydberg states. Section 2 presents the theoretical procedure adopted in this work. In Section 3, we present and discuss the results obtained, compared to available literature data.

2 Theory

2.1 Brief description of the MAOT formalism

In the framework of the Modified Atomic Orbital Theory (MAOT), total energy of a $(\nu\ell)$-given orbital is expressed in the form [19, 20]

$$E(\nu\ell) = -\frac{[Z-\sigma(\ell)]^2}{\nu^2}. \tag{1}$$

For an atomic system of several electrons M, the total energy is given by (in Rydberg):

$$E = -\sum_{i=1}^{M}\frac{[Z-\sigma_i(\ell)]^2}{\nu_i^2}.$$

With respect to the usual spectroscopic notation $(N\ell,n\ell')^{2S+1}L^{\pi}$, this equation becomes

$$E=-\sum_{i=1}^{M}\frac{[Z-\sigma_i(^{2S+1}L^{\pi})]^2}{\nu_i^2}. \tag{2}$$

In the photoionisation of atoms and ions, energy resonances are generally measured relatively to the E_∞ converging limit of a given $(^{2S+1}L_J)nl$ - Rydberg series. For these states, the general expression of the energy resonance E_n is given by

$$E_n=E_\infty-\frac{1}{n^2}\Big\{Z-\sigma_1(^{2S+1}L_J)-\sigma_2(^{2S+1}L_J)\times\frac{1}{n}-\sigma_2^{\alpha}(^{2S+1}L_J)$$
$$\times(n-m)\times(n-q)\sum_k\frac{1}{f_k(n,m,q,s)}\Big\}^2. \tag{3}$$

In this equation, m and $q(m<q)$ denote the principal quantum numbers of the $(^{2S+1}L_J)nl$ - Rydberg series of the considered atomic system used in the empirical determination of the $\sigma_i(^{2S+1}L_J)$ - screening constants, s represents the spin of the nl- electron $(s=1/2)$, E_∞ is the energy value of the series limit generally determined from NIST atomic database, E_n denotes the corresponding energy resonance and Z represents the nuclear charge of the considered element. The only problem that one may face by using the MAOT formalism is linked to the determination of the $\sum_k\frac{1}{f_k(n,m,q,s)}$ -term. The correct expression of this term is determined iteratively by imposing general Eq. (3) to give accurate data with a constant quantum defect values along all the considered series. The value of α is generally fixed to 1 and or 2 during the iteration. The standard quantum defect expansion is given as follows

$$E_n=E_\infty-\frac{RZ_{core}^2}{(n-\delta)^2}. \tag{4}$$

In this equation, R, E_∞, Z_{core} and δ are the Rydberg constant, the converging limit, the electric charge of the core ion and the quantum defect, respectively.

2.2 Energy resonances of the $4s^24p^4(^1D_2)ns,nd$ and $4s^24p^4(^1S_0)ns,nd$ Rydberg series of Ne$^+$

Using Eq. (3), the energy positions of the $4s^24p^4(^1D_2)ns,nd$ and $4s^24p^4(^1S_0)ns,nd$ Rydberg series of Ne$^+$ are given by (in Rydberg units)

- For the $^2P_j^0\to(^1D_2)ns,nd$ transitions ($j=3/2$ or $1/2$)

$$E_n=E_\infty-\frac{1}{n^2}\Big\{Z-\sigma_1(^2P_j^0,^1D_2)-\sigma_2(^2P_j^0,^1D_2)\times\frac{1}{n}-\sigma_2(^2P_j^0,^1D_2)\times(n-m)\times(n-q)$$
$$\Big[\frac{1}{(n+q-m+s+1)^3}+\frac{1}{(n+q-m+s+2)^4}+\frac{1}{(n+q-m+s+3)^5}\Big]\Big\}^2. \tag{5}$$

- For the ${}^2P_j^0 \to ({}^1S_0)ns,nd$ transitions ($j=3/2$ or $1/2$)

$$E_n = E_\infty - \frac{1}{n^2}\Big\{Z - \sigma_1({}^2P_j^0, {}^1S_0) - \sigma_2({}^2P_j^0, {}^1S_0) \times \frac{1}{n} - \sigma_2({}^2P_j^0, {}^1S_0) \times (n-m) \times (n-q)^2$$
$$\Big[\frac{1}{(n+q+s)^4} + \frac{1}{(n+q-m+s+2)^4} + \frac{1}{(n+m-q-s-1)^5}\Big]\Big\}^2. \tag{6}$$

- For the ${}^2P_{3/2}^0 \to ({}^3P_2)np$ transitions

$$E_n = E_\infty - \frac{1}{n^2}\Big\{Z - \sigma_1({}^2P_{3/2}^0, {}^1P_2) - \sigma_2({}^2P_{3/2}^0, {}^1P_2) \times \frac{1}{n} - \sigma_2({}^2P_{3/2}^0, {}^1P_2) \times (n-m) \times (n-q)^2$$
$$\Big[\frac{1}{(n+q-m+s)^4} + \frac{1}{(n+q-m+s-1)^4} + \frac{1}{(n+m-q-s)^5}\Big]\Big\}^2. \tag{7}$$

The uncertainties $(\Delta\sigma_i)$ in the screening constants and those in the energy resonances (ΔE) are determined as follows.

$$\Delta\sigma = \sqrt{\frac{(\sigma-\sigma^+)^2 + (\sigma-\sigma^-)^2}{2}}, \tag{8}$$

$$\Delta E_n = \frac{|E_n(\sigma_1,\sigma_2) - E_n(\sigma_1^+,\sigma_2^+)| + |E_n(\sigma_1,\sigma_2) - E_n(\sigma_1^-,\sigma_2^-)|}{2}. \tag{9}$$

If E_n^{exp} denotes the experimental energy position and ΔE_n^{exp} the associated uncertainty, one can get the $\sigma_1^\pm,\sigma_2^\pm$ - fitting parameters from the following relation

$$E_n(\sigma_1^\pm,\sigma_2^\pm) = E_n^{exp} \pm \Delta E_n^{exp}. \tag{10}$$

For sake of more clarifications, let us move on calculating the uncertainties $(\Delta\sigma_i)$ in the screening constants and those in the energy resonances (ΔE) for the $({}^1D_2)ns,nd$ $(j=3/2)$ Rydberg series. From the ALS measurements of Covington *et al.*, [3], we get (in eV) $E_{exp}[({}^1D_2)7s,7d] = 42.636 \pm 0.005 (m=7)$ and $E_{exp}[({}^1D_2)8s,8d] = 43.047 \pm 0.005 (q=8)$. Using $E_\infty = 44.167$, $E_{exp}[({}^1D_2)7s,7d] = 42.636$, $E_{exp}[({}^1D_2)8s,8d] = 43.047$ and 1 $Ry = 13.60569$ eV for energy conversion, Eq. (5) gives

$$\sigma_1 = 8.074663042; \quad \sigma_2 = -2.959672873. \tag{11}$$

For the $\sigma_1^\pm$, $\sigma_2^\pm$ - fitting parameters we get taking into account Eq. (10)

$$\begin{cases} E_7(\sigma_1^+,\sigma_2^+) = 42.636 + 0.005, \\ E_8(\sigma_1^+,\sigma_2^+) = 43.047 + 0.005, \end{cases} \qquad \begin{cases} E_7(\sigma_1^-,\sigma_2^-) = 42.636 - 0.005, \\ E_8(\sigma_1^-,\sigma_2^-) = 43.047 - 0.005. \end{cases}$$

Using these data, Eq. (5) provides

$$\begin{cases}\sigma_1^+ = 8.088834019, \\ \sigma_2^+ = -3.032007413, \end{cases} \qquad \begin{cases}\sigma_1^- = 8.060539735, \\ \sigma_2^- = -2.887628206. \end{cases} \tag{12}$$

Using the results (11) and (12), we obtain from Eq. (8)

$$\Delta\sigma_1 = 0.014, \quad \Delta\sigma_2 = 0.072.$$

The fitting parameters are then expressed with the correct digits as follows

$$\sigma_1 = 8.075 \pm 0.014, \quad \sigma_2 = -2.960 \pm 0.072. \tag{13}$$

As far as the uncertainties in the energy resonances are concerned, they are obtained from Eq. (9) using (11) and (12) for $n=7$ and $n=8$. The calculations for the other Rydberg series are of similar. The results found using the ALS data of Covington *et al.* [3] are quoted in Table 1.

Table 1: Screening constants values obtained using Eqs. (5), (6) and (7). The E_n -ALS resonance energies for the $(^1D_2,^1S_0)ns,nd$ series are calibrated to ± 0.005 eV and those of the $(^1P_2)ns$ series are estimated to be ± 0.010 eV. The energy limits are taken from [25].

Transitions	Levels	m	q	E_n	E_∞	σ_1	σ_2
$^2P^\circ_{3/2} \to ^1D_2ns,nd$	$(^1D_2)7s,7d$	7	-	42.636	44.167	8.075 ± 0.014	-2.960 ± 0.072
	$(^1D_2)8s,8d$	-	8	43.047			
$^2P^\circ_{1/2} \to ^1D_2ns,nd$	$(^1D_2)7s,7d$	7	-	42.539	44.070	8.083 ± 0.014	-3.017 ± 0.072
	$(^1D_2)8s,8d$		8	42.951			
$^2P^\circ_{3/2} \to ^1S_0ns,nd$	$(^1S_0)5s,5d$	5	-	44.383	47.875	8.107 ± 0.007	-3.201 ± 0.027
	$(^1S_0)6s,6d$	-	6	45.650			
$^2P^\circ_{1/2} \to ^1S_0ns,nd$	$(^1D_2)5s,5d$	5	-	44.287	47.778	8.102 ± 0.007	-3.174 ± 0.027
	$(^1D_2)6s,6d$		6	45.552			
$^2P^\circ_{3/2} \to ^3P_2np$	$(^3P_2)3p$	3	-	56.490	66.292	8.158 ± 0.006	-2.114 ± 0.014
	$(^3P_2)4p$		4	61.515			

3 Results and discussion

Tables 2-6 present comparisons of the present results with the Advanced Light Source (ALS) experimental data of Covington *et al.*, [3] and with the Screening constant by unit nuclear charge (SCUNC) calculations of Faye *et al.*, [15]. The energy resonances obtained are analyzed using the standard quantum-defect expansion formula given by Eq. (4). For all the Rydberg series investigated, it is seen that the present calculations agree well with the both experimental data [3] and theoretical values [15]. The present quantum defect is almost constant along each series up to $n = 20$ and beyond decreases slowly.

Table 2: Energy resonances (E) and quantum defect (δ) for the $2s^22p^4(^1D_2)ns,nd$ Rydberg series observed in the photoionization spectra originating from the $2s^22p^5\ ^2P^\circ_{3/2}$ ground state of Ne$^+$. The present results (MAOT) are compared to the Advanced Light Source (ALS) data of Covington *et al.*, [3] and to the SCUNC calculations of Faye *et al.*, [15].

	MAOT	SCUNC	ALS	MAOT	SCUNC	ALS
n	E(eV)			δ		
7	42.6364 (50)	42.6336 (50)	42.636 (5)	1.04	1.04	1.04
8	43.0473 (50)	43.0452 (50)	43.047 (5)	1.03	1.03	1.03
9	43.3106 (45)	43.3083 (46)	43.311 (5)	1.03	1.04	1.03
10	43.4900 (40)	43.4886 (41)	43.494 (5)	1.03	1.04	1.01
11	43.6181 (35)	43.6178 (36)	43.627 (5)	1.04	1.05	0.96
12	43.7130 (31)	43.7134 (32)	43.723 (5)	1.05	1.05	0.93
13	43.7852 (27)	43.7861 (28)	43.796 (5)	1.06	1.05	0.89
14	43.8415 (24)	43.8427 (25)	43.851 (5)	1.07	1.05	0.88
15	43.8862 (21)	43.8875 (23)	43.896 (5)	1.08	1.04	0.83
16	43.9224 (19)	43.9237 (20)	43.932 (5)	1.08	1.04	0.78
17	43.9521 (17)	43.9533 (18)	43.963 (5)	1.09	1.04	0.67
18	43.9767 (16)	43.9778 (17)	43.986 (5)	1.09	1.04	0.66
19	43.9973 (14)	43.9983 (15)	44.007 (5)	1.09	1.04	0.56
20	44.0148 (13)	44.0156 (14)	44.025 (5)	1.09	1.04	0.42
21	44.0298 (12)	44.0304 (13)	44.041 (5)	1.09	1.04	0.22
22	44.0426 (11)	44.0432 (12)	44.053 (5)	1.08	1.04	0.15
23	44.0538 (10)	44.0542 (11)	44.063 (5)	1.07	1.04	0.12
24	44.0635 (9)	44.0638 (10)	44.073 (5)	1.07	1.03	-0.06
25	44.0721 (9)	44.0722 (9)	44.080 (5)	1.06	1.03	-0.01
26	44.0796 (8)	44.0797 (9)		1.05	1.03	
27	44.0863 (8)	44.0863(8)		1.04	1.03	
28	44.0922 (7)	44.0922 (8)		1.02	1.03	
29	44.0975 (7)	44.0974(7)		1.01	1.03	
30	44.1023 (6)	44.1021(7)		0.99	1.03	
…						
∞	44.1670					

This explain why the calculations are limited to $n=30$. The good agreement between the present calculations and the high-resolution ALS measurements of Covington *et al.*, [3] may demonstrate the accuracy of the MAOT predictions and subsequently its validity to investigated Rydberg series of atoms and ionic species. In addition, for some resonances, the ALS energy resonances and quantum defects have not been well resolved and this may probably due to interference between series. For example, it is the case of the $2s^22p^4(^1D_2)ns,nd$ Rydberg series originating from the $2s^22p^5\ ^2P^\circ_{1/2}$ ground state as quoted in Table 3 for $n=12,15,18,20,21,22,23$, and 24. For these states, it is shown that the

Table 3: Same as in Table 2 for the $2s^22p^4(^1D_2)ns,nd$ Rydberg series originating from the $2s^22p^5\ ^2P^{\circ}_{1/2}$ metastable state of Ne^+.

	MAOT	SCUNC	ALS	MAOT	SCUNC	ALS
n	E(eV)			δ		
7	42.5392 (50)	42.5409 (50)	42.539 (5)	1.04	1.03	1.04
8	42.9511 (50)	42.9524 (50)	42.951 (5)	1.03	1.02	1.03
9	43.2148 (46)	43.2164 (46)	43.215 (5)	1.02	1.02	1.02
10	43.3943 (41)	43.3958 (41)	43.399 (5)	1.03	1.02	0.99
11	43.5224 (36)	43.5238 (36)	43.528 (5)	1.03	1.02	0.98
12	43.6171 (32)	43.6184 (32)		1.04	1.02	
13	43.6893 (28)	43.6905 (28)	43.698 (5)	1.04	1.02	0.90
14	43.7455 (25)	43.7466 (25)	43.755 (5)	1.05	1.03	0.86
15	43.7902 (22)	43.7911 (22)		1.05	1.03	
16	43.8263 (20)	43.8271 (20)	43.836 (5)	1.06	1.03	0.75
17	43.8559 (18)	43.8565 (18)	43.866 (5)	1.06	1.04	0.67
18	43.8804 (16)	43.8809 (16)		1.06	1.04	
19	43.9010 (15)	43.9013 (15)	43.911 (5)	1.05	1.04	0.50
20	43.9185 (14)	43.9186 (14)		1.05	1.04	
21	43.9334 (13)	43.9334 (12)	43.944 (5)	1.04	1.04	0.22
22	43.9462 (12)	43.9461 (11)		1.04	1.04	
23	43.9573 (11)	43.9571 (11)		1.03	1.04	
24	43.9670 (10)	43.9667 (10)	43.976 (5)	1.01	1.04	-0.06
25	43.9755 (9)	43.9752 (9)		1.00	1.05	
26	43.9830 (9)	43.9826 (8)		0.99	1.05	
27	43.9897 (8)	43.9892 (8)		0.97	1.05	
28	43.9956 (8)	43.9951 (7)		0.96	1.05	
29	44.0009 (7)	44.0003 (7)		0.94	1.05	
30	44.0056 (7)	44.0051 (7)		0.92	1.05	
…						
∞	44.0700					

present MAOT calculations give confidence to the accuracy of the recent SCUNC predictions [15]. Besides, it should be underlined the excellent agreements between theories up to $n=30$. These agreements are due to the fact that the MAOT and SCUNC methods are both semi-empirical quantum models based on the determination of fitting parameters using high-resolution measurements that incorporate relativistic effects. But, these two methods have not the same analytical structure and this may be explained briefly. In the framework of the SCUNC formalism, the energy resonance of a given Rydberg series is expressed in the following shape [14, 15, 23]

$$E_n = E_\infty - \frac{Z_0^2}{n^2}\left\{1-\beta(Z_0,{}^{2S+1}L_J,n,s,\mu,\nu)\right\}^2. \tag{14}$$

Table 4: Same as in Table 2 for the $2s^22p^4(^1S_0)ns,nd$ Rydberg series originating from the $2s^22p^5\ ^2P^{\circ}_{3/2}$ ground state of Ne^+.

	MAOT	SCUNC	ALS	MAOT	SCUNC	ALS
n	E(eV)			δ		
5	44.3826 (50)	44.3846 (50)	44.383 (5)	1.05	1.05	1.05
6	45.6498 (50)	45.6507 (50)	45.650 (5)	1.05	1.05	1.05
7	46.3357 (44)	46.3353 (44)	46.335 (5)	1.05	1.05	1.06
8	46.7467 (37)	46.7470 (37)	46.746 (5)	1.06	1.05	1.06
9	47.0130 (31)	47.0135 (31)	47.014 (5)	1.05	1.05	1.05
10	47.1953 (27)	47.1956 (27)	47.196 (5)	1.05	1.05	1.05
11	47.3254 (23)	47.3255 (23)	47.326 (5)	1.05	1.05	1.04
12	47.4214 (20)	47.4214 (20)	47.425 (5)	1.05	1.04	1.00
13	47.4943 (17)	47.4942 (17)	47.499 (5)	1.04	1.04	0.97
14	47.5509 (15)	47.5508 (15)		1.04	1.04	
15	47.5957 (13)	47.5956 (13)		1.04	1.04	
16	47.6318 (12)	47.6318 (12)		1.04	1.04	
17	47.6614 (11)	47.6613 (11)		1.04	1.04	
18	47.6859 (9)	47.6858 (9)		1.04	1.04	
19	47.7064 (9)	47.7063 (9)		1.03	1.04	
20	47.7237 (8)	47.7236 (8)		1.03	1.04	
21	47.7386 (7)	47.7384 (7)		1.03	1.04	
22	47.7513 (7)	47.7511 (7)		1.02	1.04	
23	47.7624 (6)	47.7622 (6)		1.02	1.04	
24	47.7720 (6)	47.7718 (6)		1.01	1.04	
25	47.7805 (5)	47.7802 (5)		1.00	1.04	
26	47.7880 (5)	47.7877 (5)		0.99	1.04	
27	47.7946 (4)	47.7943 (4)		0.98	1.04	
28	47.8005 (4)	47.8001 (4)		0.97	1.04	
29	47.8058 (4)	47.8054 (4)		0.96	1.04	
30	47.8105 (4)	47.8101 (4)		0.95	1.04	
…	…	…	…			
∞	47.8750					

In Eq. (14), ν and μ $(\mu > \nu)$ denote the principal quantum numbers of the $(^{2S+1}L_J)nl$ Rydberg series used in the empirical determination of the f_i - screening constants, s represents the spin of the nl- electron $(s=1/2)$, E_∞ is the energy value of the series limit, En denotes the resonance energy and Z_0 represents the atomic number. The β-parameters are screening constants by unit nuclear charge expanded in inverse powers of Z_0 and given by

$$\beta\left(^{2S+1}L_J,n,s,\mu,\nu\right) = \sum_{k=1}^{q} f_k \left(\frac{1}{Z_0}\right)^k. \qquad (15)$$

Table 5: Same as in Table 2 for the $2s^22p^4(^1S_0)ns,nd$ Rydberg series originating from the $2s^22p^5\ ^2P^{\circ}_{1/2}$ ground state of Ne^+.

	MAOT	SCUNC	ALS	MAOT	SCUNC	ALS
n	E(eV)			δ		
5	44.2867 (50)	44.2834 (50)	44.287 (5)	1.05	1.05	1.05
6	45.5518 (50)	45.5500 (50)	45.552 (5)	1.06	1.06	1.06
7	46.2373 (44)	46.2453 (44)	46.238 (5)	1.06	1.04	1.06
8	46.6482 (37)	46.6514 (37)	46.650 (5)	1.06	1.05	1.05
9	46.9146 (31)	46.9154 (31)	46.918 (5)	1.06	1.06	1.05
10	47.0970 (27)	47.0968 (27)	47.098 (5)	1.06	1.06	1.05
11	47.2273 (23)	47.2268 (23)	47.229 (5)	1.06	1.06	1.04
12	47.3234 (20)	47.3229 (20)		1.06	1.06	
13	47.3963 (17)	47.3960 (17)	47.401 (5)	1.06	1.06	0.99
14	47.4530 (15)	47.4528 (15)	47.454 (5)	1.06	1.06	1.04
15	47.4980 (13)	47.4979 (13)		1.06	1.06	
16	47.5342 (12)	47.5342 (12)		1.06	1.06	
17	47.5638 (11)	47.5639 (11)		1.06	1.06	
18	47.5883 (10)	47.5884 (10)		1.06	1.06	
19	47.6089 (9)	47.6090 (9)		1.06	1.05	
20	47.6263 (8)	47.6264 (8)		1.06	1.05	
21	47.6412 (7)	47.6412 (7)		1.06	1.05	
22	47.6539 (7)	47.6540 (7)		1.06	1.05	
23	47.6650 (6)	47.6651 (6)		1.05	1.05	
24	47.6747 (6)	47.6747 (6)		1.05	1.05	
25	47.6832 (5)	47.6831 (5)		1.04	1.05	
26	47.6907 (5)	47.6906 (5)		1.03	1.05	
27	47.6973 (4)	47.6972 (4)		1.03	1.05	
28	47.7032 (4)	47.7031 (4)		1.02	1.04	
29	47.7085 (4)	47.7084 (4)		1.01	1.04	
30	47.7133 (4)	47.7131 (4)		1.00	1.04	
…						
∞	47.7780					

where $f_k = f_k\left(^{2S+1}L_J, n, s, \mu, \nu\right)$ are parameters to be evaluated empirically.

Let us express Eq. (3) in the same form than Eq. (14). We get

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{\sigma_1(^{2S+1}L_J)}{Z} - \frac{\sigma_2(^{2S+1}L_J)}{Z} \times \frac{1}{n} - \frac{\sigma_2^{\alpha}(^{2S+1}L_J)}{Z} \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n,m,q,s)}\right\}^2 \tag{16}$$

Table 6: Same as in Table 2 for the $2s^22p^5(^1P_2)np$ Rydberg series originating from the $2s^22p^5\ ^2P^{\circ}_{3/2}$ ground state of Ne^+.

	MAOT	SCUNC	ALS	MAOT	SCUNC	ALS
n		E(eV)			δ	
3	56.4876 (100)	56.4888 (100)	56.490 (10)	0.64	0.64	0.64
4	61.5136 (100)	61.5143 (100)	61.515 (10)	0.63	0.62	0.62
5	63.4633 (77)	63.4595 (76)	63.459 (10)	0.61	0.62	0.62
6	64.4120 (58)	64.4173 (58)	64.420 (10)	0.62	0.61	0.61
7	64.9508 (44)	64.9595 (45)	64.956 (10)	0.63	0.61	0.62
8	65.2873 (35)	65.2962 (36)	65.294 (10)	0.64	0.61	0.62
9	65.5117 (28)	65.5196 (29)	65.520 (10)	0.65	0.61	0.60
10	65.6691 (23)	65.6753 (24)	65.673 (10)	0.65	0.61	0.62
11	65.7837 (20)	65.7883 (20)	65.786 (10)	0.65	0.61	0.63
12	65.8697 (17)	65.8728 (17)	65.874 (10)	0.65	0.61	0.59
13	65.9358 (14)	65.9376 (15)		0.64	0.61	
14	65.9878 (13)	65.9885 (13)		0.63	0.61	
15	66.0293 (11)	66.0292 (11)		0.61	0.61	
…						
∞	66.2920					

Using Eq. (15), one can rewrite Eq. l(14) in the form

$$E_n = E_\infty - \frac{Z^2}{n^2}\left\{1 - \frac{f_1(^{2S+1}L_J,n,s,\mu,\nu)}{Z_0} - \frac{f_2(^{2S+1}L_J,n,s,\mu,\nu)}{Z_0^2} + \sum_{k=3}^{q} f_k(^{2S+1}L_J,n,s,\mu,\nu)\left(\frac{1}{Z_0}\right)^k\right\}^2. \tag{17}$$

Comparison of these two formulas shows clearly the differences between the MAOT (16) and the SCUNC (17) formalisms.

4 Conclusions

The energy positions of the $2s^22p^4(^1D_2)ns,nd$, $2s^22p^4(^1S_0)ns,nd$ and $2s^2p^5(^3P_2)np$ Rydberg series originating from the $2s^22p^5\ ^2P_{1/2}$ metastable and from the $2s^22p^5\ ^2P_{3/2}$ ground state of Ne^+ are reported in this paper up to $n=30$ applying the MAOT formalism. On the whole, the present results agree well with the ALS measurements of Covington *et al.* [3] and with the Screening constant by unit nuclear charge calculations of Faye *et al.*, [15]. As explained by Robicheaux and Geene [24], for halogen atoms, only the very sophisticated eigenchannel R-matrix approach has been able to satisfactorily reproduce the experimental spectra. The very good agreement between the present calculations and the ALS measurements, points out that the MOAT formalism can be used fruitfully to assist experimentalists for the identification of a wealth of resonance structures observed during the running set up. In addition, one can apply the present MAOT formalism to investigate the photoionization of other ionic neon species such as Ne^{2+}, Ne^{3+}, and Ne^{4+} who contribute to the opacity in the atmospheres of the central stars of planetary nebulas.

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