

Research Article

Calculations of Resonances Energies of the Ne Atom, Ne-like Na^+ , Mg^{2+} , and Ne^+ Ions, Framework of the Modified Atomic Orbital Theory

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Abstract

In the literature, there are several theoretical and experimental methods for calculating the resonance energies and natural widths of atomic systems. For the $1s^2 2s 2p^6 n p$ P^1 series of Ne, Na^+ , Mg^{2+} , and the $1s 2s^2 2p^5 n p$ P^1 series of Ne^+ , various methods have been employed. In this present work, resonance energies and width of the $1s^2 2s 2p^6 n p$ P^1 series of the Ne, Na^+ , Mg^{2+} , and $1s 2s^2 2p^5 n p$ P^1 of Ne^+ ions are calculated. The energies are calculated in the framework of the Modified Atomic Orbital Theory (MAOT). The results obtained compared very well with theoretical and experimental literature values. The possibility to use the MAOT formalism report rapidly with an excellent accuracy the position of the resonances as well as their width within simple analytical formulae is demonstrated. It is demonstrated that the MAOT-method can be used to assist fruitfully experiments for identifying narrow resonance energies. Thus, our results can be used as reference data for the interpretation of atomic spectra for the diagnosis of astrophysical and laboratory plasma. Through this method new values of these energies are reported going up to $n=40$. These excellent agreements between theory and experiments indicate that the MAOT formalism can be used to report accurate high-lying excited Rydberg series of atomic species for the diagnostic and the modeling of astrophysical or laboratory plasmas.

Keywords

Photoionization, Resonance Energies, Width, Modified Atomic Orbital Theory, Rydberg Series, Synchrotron Radiation

1. Introduction

The emission and absorption of electromagnetic radiation by matter are strongly dependent on photon energy [1]. The resulting spectral patterns are unique to each atom and its various charge states. Therefore, radiation spectra from astrophysical objects or laboratory plasmas can provide insights into the abundances of elements, their ionization stages, and

the properties of the environment where these elements are found [2].

Depending on the temperature and ambient radiation field of their physical environment, neon atoms exist in different charge states q covering the full range from $q=0$ to $q=10$. Terrestrial observatories can access spectral information from

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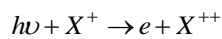
beyond the earth's atmosphere only at wavelengths exceeding about 100 nm [1]. Neon lines observed in astrophysical spectra, such as from planetary nebulae [5-7] and galaxies [8], can be used for the diagnostics of the objects.

However, neon ions, due to their structure and various applications in laboratory experiments, astrophysics, and plasma physics, have been the subject of several experimental and theoretical studies.

Autoionization is thus essentially a consequence of electron correlation and requires a many-body theory for its calculation. Studies of the autoionization resonances in noble-gas atoms [8] have long attracted experimental and theoretical scrutiny. The significant cosmic abundance of neon like highly charged ions (HCI) and other similar atomic or ionic many-electron systems has drawn special attention to their photoionization, with particular emphasis upon the asymmetric line profiles exhibited by the autoionization resonances [7, 9, 10]. High-resolution studies with an accuracy of 3 meV in the photon energy range of 44 to 53 eV, revealing new relativistic features of highly excited resonances of Neon converging to different fine-structure thresholds $2p4 (^3P)3s^2P$ and $2p4 (^3P)3p^2P$ states of Ne^+ , were conducted by Schulz et al. [9]. The Screening Constant by Unit Nuclear Charge (SCUNC) formalism [3] reported accurate photoabsorption data Ne and of Ne-like Na^+ , Mg^{2+} , Al^{3+} , Si^{4+} , P^{5+} , S^{6+} , and Cl^{7+} ions. Furthermore, others studied the single, double, and triple photoionization of Ne^+ ions by single photons at the synchrotron radiation source PETRA III in Hamburg [1].

These authors reported natural widths and photon energies of the Ne^+ $1s2s^22p5 np^1P_1$ Levels ($n=3, 4, 5, 6$) from the ground state of Ne [1].

Photoionization is a well known process and described in literature [4]. A brief outline is given below for the guidance of the readers. Photoionization occurs directly:



Moreover, the photoexcitation of the Ne ($1s^2s^2p^6 S$) ground state in the photon energy range of 840-930 eV can lead to the excitation of a single K-shell electron [1]. The calibration measurements allowed us to further investigate photoabsorption by neutral neon as part of the present work on Ne^+ ions.

The objective of this study is only focused on the photoionization of neon like Na^+ , Mg^{2+} and Ne^+ ions. We applied the MAOT formalism [12, 13] to report resonance energies

and widths of the $1s^22s2p^6 np^1P_1$ series of Ne and Ne-like Na^+ and Mg^{2+} . We also report the resonance energy $1s2s^22p^5 np^1P_1$ of Ne^+ via the same formalism.

In this paper, after providing a brief description of the MAOT procedure, we present the resonance energy calculations for the Rydberg series of Ne and Ne-like ions, as well as the effective quantum number n . The obtained results will then be displayed and discussed. Finally, a conclusion will be drawn.

2. Theory

2.1. General Formalism of the MOAT Method

The bases of the MAOT formalism will be presented in detail in this paper, and the total energy of a given orbital (νl) is expressed in Rydberg units [12, 13].

$$E(\nu l) = -\frac{[Z - \sigma(l)]^2}{\nu(l)^2} \quad (1)$$

In Eq. (1), Z stands for the atomic number, σ is the screening constant relative to the electron occupying the νl orbital, ν and l denotes respectively the principal quantum number and the orbital quantum number. However, the doubly excited states (DES) in two electron systems are labelled as $(Nl, nl')^{2S+1}L^\pi$. For the previous term, N denotes the quantum number of the inner electron and n that of the outer electron, their respective orbital quantum numbers are l and l' , the total spin is represented by S , L is the total angular momentum, and the parity of the system is represented by π . For the $(Nl, nl')^{2S+1}L^\pi$ doubly excited states, the total energy of an atomic system of many M electrons is expressed as follows [12, 13]:

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

In the photoionization study, the general expression of the resonance energy E_n for $(^{2S+1}L_J)nl$ - Rydberg series is given by (in Rydberg units). For these states [12, 13]

$$E_n = E_\infty - \frac{1}{n^2} \left\{ Z - \sigma_1(^{2S+1}L_J) - \sigma_2(^{2S+1}L_J) \times \frac{1}{n} - \sigma_2^\alpha(^2P_{3/2}, ^1D_2) \times (n-m) \times (n-q) \sum_k \frac{1}{f_k(n, m, q, s)} \right\}^2 \quad (3)$$

In this equation, m and q (with $m < q$) represent the principal quantum numbers of the $(^{2S+1}L_J)nl$ Rydberg series of the atomic system under study, used for the empirical determination of the

$\sigma_i(^{2S+1}L_J)$ screening constants, s denotes the spin of the nl -electron ($s = 1/2$), E_∞ is the energy value of the series limit, typically obtained from the NIST atomic database, and Z rep-

resents the nuclear charge of the element in question. The only challenge encountered when using the MAOT formalism is

related to the determination of the $\sum_k \frac{1}{f_k(n, m, q, s)}$ term [12, 13].

The exact expression of this term is derived iteratively by applying the general equation (3) to generate accurate data with constant quantum defect values across all the studied series. During the iteration, the value of α is set to either 1 or 2. The quantum defect is determined using the standard formula

$$E_n = E_\infty - \frac{RZ^2}{(n - \delta)^2} \quad (4)$$

In this equation, R refers to the Rydberg constant, E_∞ represents the convergence limit, Z_{core} denotes the electric charge of the core ion, and δ indicates the quantum defect. As for the natural widths, they are expressed in Rydberg units as stated in [12].

$$\Gamma_n = \frac{1}{n^2} \left\{ Z - \sigma_1'(^{2S+1}L_J) - \sigma_2'(^{2S+1}L_J) \times \frac{1}{n} - \sigma_2'^{(2P_{3/2}^0, ^1D_2)} \times (n-m) \times (n-q) \sum_k \frac{1}{f_k'(n, m, q, s)} \right\}^2 \quad (5)$$

2.2. Resonance Energy of the $1s2s^22p^5$ np 1P_1 Series of Ne^+

$$E_n = E_\infty - \frac{1}{n^2} \left\{ Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n-m+q+s+1)^6} + \frac{1}{(n+q-m+6s)^6} + \frac{1}{(n+q-m+3s+3)^8} \right] \right\}^2 \quad (6)$$

2.3. Resonance Energy of the $1s^22s2p^4$ (1D) $3s$ (2D) np 1P and $1s^22s2p^4$ (3P) $3p$ (2P) ns 1P Series of Ne

For $1s^22s2p^4$ (1D) $3s$ (2D) np 1P

$$E_n = E_\infty - \frac{1}{n^2} \left\{ Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n-m+q+s+1)^5} + \frac{1}{(n+q-m+2s+2)^6} + \frac{1}{(n+q-m+3s+3)^7} \right] \right\}^2 \quad (7)$$

For $1s^22s2p^4$ (3P) $3p$ (2P) ns 1P

$$E_n = E_\infty - \frac{1}{n^2} \left\{ Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n-m+q+s-2)^3} + \frac{1}{(n+q-m+3s)^3} + \frac{1}{(n+q-m+4s+3)^7} \right] \right\}^2 \quad (8)$$

2.4. Resonance Energies and of the Natural Widths of the $1s^22s2p^6$ np 1P_1 Series of Na^+ , Mg^{2+} (in Rydberg Units)

Resonance energies are given by the simple formula

$$E_n = E_\infty - \frac{1}{n^2} \left\{ Z - \sigma_1 - \sigma_2 \times \frac{1}{n} - \sigma_2 \times (n-m) \times (n-q) \times \left[\frac{1}{(n-m+q+1.5s+2)^3} + \frac{1}{(n+q-m+4s+2.8)^3} + \frac{1}{(n+q-m+3s+3)^3} \right] \right\}^2 \quad (9)$$

The natural widths are given by

In addition, using (5), we express the natural width as follows

$$\Gamma_n = \frac{1}{n^2} \left\{ Z - \sigma_1(^{2S+1}L_J) - \sigma_2(^{2S+1}L_J) \times \frac{1}{n} + \sigma_2'^{(2S+1}L_J) \times (n-m) \times (n-q) \times \left[\frac{1}{(n+q-m+s+1)^3} + \frac{1}{(n+q-m+s+2)^4} + \frac{1}{(n+q-m+s+3)^5} \right] \right\}^2 \quad (10)$$

For all other series, the natural widths are given in the same form as the equation.

3. Results and Discussion

In Equations (7, 8, 9), and (10), the σ_i screening constant data, empirically evaluated, are obtained using the data from Sakho [3] and Equation (6) from synchrotron radiation measurements of Müller et al. [1]. The present paper results are compared with those from existing theoretical and experimental literature. Each result is mentioned in a table along with its comparisons.

Tables 1 and 3 list resonance energy of the $1s^2 2s 2p^4 (^1D) 3s (^2D) np^1 P$ and $1s^2 2s 2p^4 (^3P) 3p (^2P) ns^1 P$ series of Ne respectively. In this section, our results have been compared with those obtained by the following authors: Theoretically, first with the results from the Screening Constant by Unit Nuclear Charge (SCUNC) method [3], and then with results from Numerical Calculations (NC) [11]; experimentally, with results from Synchrotron Radiation (SR) [11], and then from Photoabsorption (PA) [15]. The energy value of the series limit is and the σ_i screening constants in Eqs. (7, 8) taken from Sakho [3]. For the doubly $2s 2p^4 (^1D) 3s (^2D) np^1 P$ excited states of Ne ($m=3$) and ($q=4$) levels equal to 48.9066 eV, and 50.5600 eV, respectively. We get $\sigma_1 = 8,9621$ and $\sigma_2 = -1,2570$. For the doubly $2s 2p^4 (^3P) 3p (^2P) ns^1 P$ excited states of Ne ($m=4$) and ($q=5$) levels equal to 50.7601 eV, and 51.8926 eV respectively. We get $\sigma_1 = 9,3227$ and $\sigma_2 = -3,9005$.

For doubly $2s 2p^4 (^3P) 3p (^2P) ns^1 P$ and $2s 2p^4 (^3P) 3p (^2P) ns^1 P$ excited states, the MAOT results listed in Tables 1 and 3 are seen to agree very well with both the quoted experimental and theoretical data up to $n = 9$ between MAOT and PA from Photoabsorption experiments of Codling et al [15], to $n=16$ between MAOT and (SR) from Synchrotron radiation experiments of Schulz et al. [11]. The energy difference $\Delta E = E_{MAOT} - E_{PA}$ or $\Delta E = E_{MAOT} - E_{SR}$ between these levels values at 0,016 eV and 0,014 eV respectively. New theoretical values were found, ranging from $n=40$. In general, experiments and theories are in perfect agreement.

The effective quantum number n^* of the doubly $2s 2p^4 (^1D) 3s (^2D) np^1 P$, and $2s 2p^4 (^3P) 3p (^2P) ns^1 P$ excited states of Ne is presented in Tables 2 and 4, respectively. In pure LS coupling where relativistic effects can be neglected, the effective quantum number is simply $n^* = n - \delta$, with δ the quantum defect of the resonance. with δ the quantum defect of the resonance. Comparison indicates a very good agreement between the MAOT calculations and the quoted theoretical and experimental values up to $n = 20$. However, the jj coupling, where the quantum defect is given by

$$\delta_{nlj} = n - n^* + (j+1) - \left[(j+1)^2 - (z\alpha)^2 \right]^{1/2}, \text{ with } z \text{ being the}$$

asymptotic charge seen by the photoelectron and α the fine-structure constant [16], better describes the resonance parameters in this work through correlation effects. This better explains some MOAT values in Tables 2 and 4.

Table 5 and 6 list resonance energy and natural width of the $2s 2p^6 np^1 P_1$ series of Na^+ and Mg^{2+} . For Na^+ and Mg^{2+} , our MOAT results are compared with the theoretical results from SCUNC [3], HPTL, high-power adjustable laser calculations of Lucatorto et al. [14], DHF calculations [16], and HVSS, high-voltage spark spectra of Kastner et al. [17].

The energy value of the series limit is and the σ_i screening constants in Eqs. (9, 10) taken from Sakho [3]. For the doubly $2s 2p^6 np^1 P_1$ excited states of Na^+ ($m=3$) and ($q=4$) levels equal to 69.950 eV, and 75.320 eV, respectively. We get $\sigma_1 = 9,1851$ and $\sigma_2 = -2,3953$. For the doubly $2s 2p^6 np^1 P_1$ excited states of Mg^{2+} ($m=3$) and ($q=4$) levels equal to 98.776 eV, and 109.004 eV, respectively. We get $\sigma_1 = 9,2064$ and $\sigma_2 = -2,6262$.

For natural width of the $2s 2p^6 np^1 P_1$ series of Na^+ and Mg^{2+} . We compare the current MAOT calculations with other theoretical and experimental calculations. The screening constants σ_i in Eq. (10) are taken from Sakho [3].

For the doubly $2s 2p^6 np^1 P_1$ excited states of Na^+ ($m=3$) and ($q=4$) levels equal to 51,56 meV, and 22,50 meV, respectively. We get $\sigma_1 = 10, 9030$ and $\sigma_2 = -0, 2642$. For the doubly $2s 2p^6 np^1 P_1$ excited states of Mg^{2+} ($m=3$) and ($q=4$) levels equal to 94,51 meV, and 43,44 meV, respectively. We get $\sigma_1 = 11,8460$ and $\sigma_2 = -0,2882$. In general, good agreement is obtained between the quoted data; and new values referring to have been cited as references for future studies. Comparison shows excellent agreements with literature calculations.

Table 7 list resonance energy of the $1s 2s^2 2p^5 np^1 P_1$ of Ne^+ . For the $1s 2s^2 2p^5 np^1 P_1$ of Ne^+ , our MOAT results are compared with those of Muler et al. [1], the photoabsorption data from Witthoeft et al. [18] and Gorczyca [19], as well as those from Juett et al. [20] and Gatuuzz et al. [21]. The energy value of the series limit is and the σ_i screening constants in Eqs. (6) are derived from the experimental data of Müller et al. [1]. For these states, ($m=3$) and ($q=4$) levels equal to 889.45 eV and 894.90 eV. We get $\sigma_1 = 8,3511$ and $\sigma_2 = -2,8382$. The energy difference $\Delta E = E_{MAOT} - E_a$ to $n = 3$ between these levels values at 0,03 eV. After comparison, we can state that our MAOT method allowed us to obtain accurate values up to $n = 20$. These values are in good agreement with those obtained from Muller's synchrotron radiation [1].

Table 1. Resonance energies (E , eV), of the doubly $2s2p^4$ (1D) $3s$ (2D) np^1P excited states of Ne. $|\Delta E_{MAOT,SR}|$ denotes the energy difference between the present MAOT calculations and the experimental data of SR.

States	Theory			Experiment		
	MAOT	SCUNC	NC	SR	PA	$ \Delta E_{MAOT,SR} $
3	48.9066	48.9066	48.9063	48.9066	48.907	0.00
4	50.5600	50.5664	50.6496	50.56	50.565	0.00
5	51.2096	51.2494	51.3049	51.262	51.276	0.05
6	51.5260	51.5632	51.5865	51.561	51.563	0.03
7	51.7025	51.7326	51.745	51.732	51.736	0.03
8	51.8105	51.8343	51.8419	51.8332	51.842	0.02
9	51.8811	51.9001	51.9047	51.8975	51.898	0.02
10	51.9298	51.9452	51.9479	-	-	-
11	51.9648	51.9773	51.9789	51.9792		0.01
12	51.9907	52.0011	52.0017	52.0032		0.01
13	52.0104	52.0192	52.0186	52.0208		0.01
14	52.0258	52.0332	52.0299	52.0348		0.01
15	52.0379	52.0444		52.0452		0.01
16	52.0478	52.0534		52.0542		0.01
17	52.0558	52.0607				
18	52.0625	52.0668				
19	52.0681	52.0719				
20	52.0728	52.0762				
21	52.0768	52.0799				
22	52.0803	52.0831				
23	52.0833	52.0858				
24	52.0859	52.0882				
25	52.0882	52.0903				
26	52.0903	52.0922				
27	52.0921	52.0938				
28	52.0937	52.0953				
29	52.0951	52.0966				
30	52.0964	52.0978				
31	52.0975					
32	52.0986					
33	52.0995					
34	52.1004					
35	52.1012					
36	52.1019					
37	52.1026					

States	Theory		Experiment			
	MAOT	SCUNC	NC	SR	PA	$ \Delta E_{MAOT,SR} $
38	52.1032					
39	52.1038					
40	52.1043					
...						
∞	52.114	52.114				

MAOT, Modified Atomique Orbital Theory, Present calculations.

SCUNC [3]; NC [11]; SR [11]; PA [15]

Table 2. Effective quantum number $n^* = n - \delta$ of the doubly $2s2p^4$ (1D) $3s$ (2D) np^1P excited states of Ne.

States	Theory		Experiment	
	MAOT	SCUNC	NC	SR
3	2.060	2.060	2.060	2.0597 (5)
4	2.959	2.965	3.049	2.963 (7)
5	3.879	3.967	4.102	3.997(12)
6	4.810	4.970	5.082	4.961(13)
7	5.750	5.972	6.078	5.970 (23)
8	6.695	6.974	7.080	6.964 (19)
9	7.644	7.976	8.075	7.933 (28)
10	8.595	8.977	9.069	-
11	9.548	9.978	10.039	10.058 (93)
12	10.503	10.979	11.039	11.10 (13)
13	11.460	11.979	11.985	12.10 (16)
14	12.417	12.980	12.771	13.13 (21)
15	13.375	13.980		14.09 (26)
16	14.335	14.981		15.12 (32)
17	15.294	15.981		
18	16.254	16.981		
19	17.214	17.982		
20	18.174	18.982		
21	19.135	19.982		
22	20.096	20.982		
23	21.057	21.982		
24	22.019	22.983		
25	22.980	23.983		
26	23.942	24.983		

States	Theory			Experiment
	MAOT	SCUNC	NC	SR
27	24.904	25.983		
28	25.866	26.983		
29	26.828	27.983		
30	27.790	28.983		
31	28.753			
32	29.715			
33	30.678			
34	31.640			
35	32.603			
36	33.566			
37	34.528			
38	35.491			
39	36.454			
40	37.417			
...				

Table 3. Resonance energies (E , eV), of the doubly $2s2p^4$ (3P) $3p$ (2P) ns 1P excited states of Ne. $|\Delta E_{MAOT,SR}|$ denotes the energy difference between the present MAOT calculations and the experimental data of SR.

States	Theory				Experiment	
	MAOT	SCUNC	NC	SR	PA	$ \Delta E_{MAOT,SR} $
	E			E		$ \Delta E $
4	50.7601	50.76	51.1834	50.76	50.749	0.00
5	51.8926	51.9271	52.0367	51.926	51.928	0.03
6	52.3724	52.3847	52.4303	52.388	52.387	0.02
7	52.6159	52.6157	52.64	52.618	-	0.00
8	52.7552	52.7485	52.7623	52.7493	52.737	0.01
9	52.8418	52.8319	52.8394	52.832	52.827	0.01
10	52.8990	52.8876	52.8916	52.8863	52.8863	0.01
11	52.9386	52.9266	52.9282	52.9243		0.01
12	52.9670	52.955	52.9549	52.9513		0.00
13	52.9881	52.9763				
14	53.0041	52.9926				
15	53.0164	53.0055				
16	53.0262	53.0157				
17	53.0340	53.0241				

States	Theory				Experiment	
	MAOT	SCUNC	NC	SR	PA	$ \Delta E_{MAOT,SR} $
	E			E		$ \Delta E $
18	53.0403	53.0309				
19	53.0455	53.0366				
20	53.0499	53.0414				
21	53.0535	53.0455				
22	53.0566	53.049				
23	53.0592	53.052				
24	53.0614	53.0547				
25	53.0634	53.0569				
26	53.0651	53.059				
27	53.0665	53.0607				
28	53.0678	53.0623				
29	53.0690	53.0637				
30	53.0700	53.065				
31	53.0709					
32	53.0717					
33	53.0724					
34	53.0731					
35	53.0737					
36	53.0742					
37	53.0747					
38	53.0751					
39	53.0756					
40	53.0759					
...						
∞	53.082					

Table 4. Effective quantum number n^* of the doubly $2s2p^4 (^3P) 3p (^2P) ns ^1P$ excited states of Ne.

States	Theory			Experiment
	MAOT	SCUNC	NC	SR
4	2.959	2.421	2.676	2.423 (3)
5	3.879	3.432	3.606	3.438(6)
6	4.810	4.417	4.567	4.444(13)
7	5.750	5.401	5.544	5.446 (24)

States	Theory			Experiment
	MAOT	SCUNC	NC	SR
8	6.695	6.388	6.580	6.443 (15)
9	7.644	7.376	7.578	7.452 (23)
10	8.595	8.366	8.576	8.447 (33)
11	9.548	9.357	9.576	9.440 (5)
12	10.503	10.350	10.574	10.40 (13)
13	11.460	11.344		
14	12.417	12.338		
15	13.375	13.333		
16	14.335	14.329		
17	15.294	15.325		
18	16.254	16.322		
19	17.214	17.318		
20	18.174	18.316		
21	19.135	19.313		
22	20.096	20.311		
23	21.057	21.309		
24	22.019	22.307		
25	22.980	23.305		
26	23.942	24.303		
27	24.904	25.301		
28	25.866	26.300		
29	26.828	27.298		
30	27.790	28.297		
31	28.753			
32	29.715			
33	30.678			
34	31.640			
35	32.603			
36	33.566			
37	34.528			
38	35.491			
39	36.454			
40	37.417			
...				

Table 5. Resonance energies (E , eV) of the $2s2p^6 np \ ^1P_1$ series of Na^+ and Mg^{2+} .

States	Na^+				Mg^{2+}			
	MAOT	SCUNC	HPTL	DHF	MAOT	SCUNC	DHF	HVSS
	E				E			
3	69.950	69.95	69.95	73.746	98.776	98.776	101.525	98.278
4	75.320	75.32	75.18		109.004	109.004		108.722
5	77.372	77.365	77.17		113.072	113.057		112.888
6	78.364	78.359	78.14		115.089	115.078		-
7	78.920	78.918	78.7		116.238	116.232		116.126
8	79.262	79.263	79.04		116.955	116.954		
9	79.489	79.491			117.434	117.436		
10	79.648	79.65			117.771	117.773		
11	79.763	79.765			118.016	118.018		
12	79.849	79.851			118.201	118.203		
13	79.915	79.917			118.343	118.344		
14	79.967	79.968			118.455	118.456		
15	80.009	80.009			118.545	118.545		
16	80.043	80.043			118.618	118.617		
17	80.070	80.07			118.678	118.677		
18	80.094	80.093			118.729	118.727		
19	80.113	80.112			118.771	118.769		
20	80.130	80.128			118.807	118.805		
21	80.144	80.142			118.838	118.835		
22	80.156	80.154			118.864	118.862		
23	80.167	80.165			118.888	118.885		
24	80.176	80.174			118.908	118.905		
25	80.184	80.182			118.926	118.922		
26	80.191	80.189			118.941	118.938		
27	80.197	80.196			118.955	118.952		
28	80.203	80.201			118.968	118.964		
29	80.208	80.206			118.979	118.975		
30	80.213	80.211			118.989	118.985		
31	80.217				118.998			
32	80.221				119.006			
33	80.224				119.014			
34	80.227				119.020			
35	80.230				119.027			

States	Na ⁺				Mg ²⁺			
	MAOT	SCUNC	HPTL	DHF	MAOT	SCUNC	DHF	HVSS
	E				E			
36	80.232				119.032			
37	80.235				119.038			
38	80.237				119.042			
39	80.239				119.047			
40	80.241				119.051			
...								
∞	80.274	80.274	80.091	83.877	119,126	119,126	122.356	118.766

HPTL [15]; DHF [8]; HVSS [16]

Table 6. Width (Γ , meV) of the $1s^2 2s 2p^6 np \ ^1P_1$ series of Ne-like ions ($Z = 11-12$).

n	Na ⁺			Mg ²⁺		
	MAOT	SCUNC	DHF	MAOT	SCUNC	DHF
	Γ	Γ	Γ	Γ	Γ	Γ
3	51.55	51.56	60	94.53	94.51	90
4	22.50	22.50		43.45	43.44	
5	12.38	12.11		24.72	24.40	
6	7.77	7.50		15.89	15.58	
7	5.31	5.09		11.05	10.80	
8	3.85	3.67		8.11	7.92	
9	2.91	2.77		6.20	6.06	
10	2.27	2.17		4.88	4.78	
11	1.81	1.74		3.94	3.87	
12	1.48	1.42		3.24	3.20	
13	1.23	1.19		2.71	2.68	
14	1.04	1.01		2.30	2.29	
15	0.89	0.86		1.97	1.97	
16	0.76			1.71		
17	0.67			1.50		
18	0.58			1.32		
19	0.52			1.17		
20	0.46			1.05		
21	0.41			0.94		

n	Na ⁺			Mg ²⁺		
	MAOT	SCUNC	DHF	MAOT	SCUNC	DHF
	Γ	Γ	Γ	Γ	Γ	Γ
22	0.37			0.85		
23	0.34			0.77		
24	0.31			0.70		
25	0.28			0.65		
26	0.26			0.59		
27	0.24			0.55		
28	0.22			0.50		
29	0.20			0.47		
30	0.19			0.44		

Table 7. Resonance energies (E , eV) of the $1s2s^22p^5\ n\ ^1P_1$ of Ne^+ ions. The very good agreement between the MAOT predictions and the recent synchrotron measurement of Müller et al. allows one to expect the MAOT quoted resonance energies for $n = 7-20$ as accurate. $|\Delta E_{p,a}|$ denotes the energy difference between the present MAOT calculations and the experimental data of Muler et al 2017.

n	Resonance energies (E , eV)						
	E ^p	E ^a	E ^b	E ^c	E ^d	E ^e	$ \Delta E_{p,a} $
3	889.45	889.945	890.40	890.40	890.40	890.40	0.50
4	894.90	894.90	895.00	895.40	895.40	895.40	0.00
5	896.96	897.10	897.20	897.30	897.30	897.30	0.14
6	897.93	897.90	898.28	899.2	899.2	899.2	0.03
7	898.46						
8	898.78						
9	898.98						
10	899.12						
11	899.22						
12	899.29						
13	899.35						
14	899.39						
15	899.43						
16	899.45						
17	899.47						
18	899.49						

n	Resonance energies (E , eV)						$ \Delta E_{p,a} $
	E^p	E^a	E^b	E^c	E^d	E^e	
19	899.51						
20	899.52						
					
∞	899.63	899.63					

p: present calculations; a: Muler et al (2017) [1]; b: Witthoef et al (2009) [18]; c: Gorczyca (2000) [19]; d: Juett et al. (2006) [20]; e: Gatuzz et al. (2015) [21].

4. Conclusion

Photoionization of neutral neon and Ne^+ ion has been successfully applied through Modified Atomic Orbital Theory (MAOT). Very high level energies as well as high natural widths have been found. The results presented in this study are in perfect agreement with the results available in the literature. These new high values will serve as a basis for interpreting the spectral lines of the neon atom in astrophysical objects and will serve as references for future theoretical and experimental studies.

Abbreviations

MAOT	Modified Atomic Orbital Theory
SCUNC	Screening Constant by Unit Nuclear Charge
DHF	Dirac-Hartree-Fock
SR	Synchrotron Radiation
PA	Photoabsorption
NC	Numerical Calculations
HPTL	High-power Adjustable Laser
HVSS	High-voltage Spark Spectra
DES	Doubly Excited States

Author Contributions

Each author contributed to improving the final version of the document.

Conflicts of Interest

The authors declare no conflicts of interest.

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