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Photoionization of Ne Atom Ions in the Framework of the Modified Atomic Orbital Theory

Research Article

I. Sakho

Department of Experimental Sciences, UFR Sciences and Technologies, University of Thiès, Thiès, Senegal
aminafatima_sakho@yahoo.fr

Abstract. We report accurate resonance energies and width of the $1s2s^2p^6np\ ^1P^1$ and $1s^22s2p^6np\ ^1P_1$ series of Ne neutral atom. Calculations are performed in the framework of the Modified atomic orbital theory (MAOT). Excellent agreements is obtained with high synchrotron radiation measurements of Schulz *et al*. [*Phys. Rev. A* **54**, 3095 (1996)] and of Müller *et al*. [*Astrophys. J.* **836**, 166 (2017)]. The high lying accurate resonance energies tabulated may be benchmarked data for interpreting spectra lines of Ne neutral atom from astrophysical objects.

Keywords. Photoioinization; Resonance energies; Width; Modified atomic orbital theory; Rydberg series; Synchrotron radiation

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1. Introduction

Photoionization process playing a key role in many high-temperature plasma environments such as those in stars and nebulae [1] and those in inertial-confinement fusion experiments [2]. In addition, the importance of Photoionization studies on atomic species is connected with the possibility to determine the ionization balances and the abundances of elements in photoionized astrophysical nebulae. Neon is known to be the sixth most abundant element in the universe and then is of great importance in astrophysics in connection with the role of neon ions in the interpretation of astronomical data from stellar objects such as gaseous nebulas [3]. In a pioneering experiment on Ne at photon energies from 44 to 64 eV, Codling *et al*. [4] resolved only some of the numerous spectral features due to their limited 12 meV resolution. Schulz *et al*. [5] performed high resolution at 3 meV in the photon energy range 44-53 eV to resolved new relativistic features of highly excited resonances of Ne converging to different fine structure threshold $2p^4(^3P)3s\ ^2P$ and $2p^4\ (^3P)3p\ ^2P$ states of Ne^+. Using the *Screening Constant by Unit Nuclear Charge* (SCUNC) formalism, Sakho [6] reported accurate Photoabsorption data of Ne and of Ne-like Na^+, Mg^{2+}, Al^{3+}, Si^{4+}, P^{5+}, S^{6+}, and Cl^{7+} ions. Recently, Müller *et al*. [7] investigated single, double, and triple photoionization of Ne^+ ions by single photons at the synchrotron radiation source PETRA III in Hamburg, Germany. These authors reported natural widths and excitation energies of the Ne ($1s2s^22p^6\ np\ ^1P_1$) Levels with ($n = 3,4,5,6$) from the ground state of Ne. Schulz *et al*. [5] shown that photoionization of the $2s^22p^6\ ^1S$ ground state of Ne is characterized at photon energies from 44 to 53 eV, by singly excited $2s2p^6np$ autoionizing Rydberg series and by overlapping doubly excited $2p^43snp$ and $2p^43pnl$ ($l = s,d$) autoionizing Rydberg series. The doubly excited resonances can be photoexcited mainly through the presence of electron correlations in the initial $2s^22p^6\ ^1S$ state. But, these series typically appear with very low intensities in the photoionization cross section. As far as the singly photo excitation of the Ne ($1s^22s^22p^6\ ^1S$) ground state is concerned, it can be describe by the following process

$$h\nu + \text{Ne}\ (1s^22s^22p^6\ ^1S) \to \text{Ne}\ (1s^22s2p^6np\ ^1P), \tag{1}$$

with $n = 3,4,5$, and via ionization

$$h\nu + \text{Ne}\ (1s^22s^22p^6\ ^1S) \to \text{Ne}^+(1s^22s2p^6\ ^2S) + e^-. \tag{2}$$

In addition, Müller *et al*. [7] shown that photo excitation of the Ne ($1s^22s^22p^6\ ^1S$) ground state in the photon energies range 840-930 eV can produce excitation of one single K-shell electron. This photo excitation can be describe by the processes

$$h\nu + \text{Ne}\ (1s^22s^22p^6\ ^1S) \to \text{Ne}\ (1s2s^22p^6np\ ^1P), \tag{3}$$

with $n = 3,4,5$, and via ionization

$$h\nu + \text{Ne}\ (1s^22s^22p^6\ ^1S) \to \text{Ne}^+(1s2s^22p^6\ ^2S) + e^-. \tag{4}$$

In this work, we focus our study to both the $1s^22s^22p^6\ ^1S \to 1s^22s2p^6np\ ^1P_1$ and $1s^22s^22p^6\ ^1S \to 1s2s^22p^6np\ ^1P_1$ transitions in Ne. The motivation is to report precise high lying resonance energies and width of the $1s2s^2p^6np\ ^1P_1$ and $1s2s^22p^6np\ ^1P_1$ series of Ne neutral atom using the Modified atomic orbital theory [8,9]. The present paper is organized as follows. Section 2 presents a brief outline of the theoretical part of the work. In Section 3, we present and discuss our results compared with the available experimental and theoretical results. In Section 4, we summarize our study and draw conclusions.

2. Theory

2.1 Brief Description of the MAOT Formalism

In the framework of the *Modified Atomic Orbital Theory* (MAOT), the resonance energy E_n relatively to the E_∞ converging limit of a given $(^{2S+1}L_J)nl$-Rydberg series in given by [8,9] (in Rydberg units)

$$E_n = E_\infty - \frac{1}{n^2}\left\{Z - \sigma_1(^{2S+1}L_J) - \sigma_2(^{2S+1}L_J)\frac{1}{n} - \sigma_2^{\alpha}(^2P^0_{3/2},\ ^1D_2)(n-m)(n-q)\sum_k \frac{1}{f_k(n,m,q,s)}\right\}^2. \tag{5}$$

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 fixed to 1 and or 2 during the iteration. As far as natural width is concerned, it is given by

$$\Gamma_n = \frac{1}{n^2}\left\{Z-\sigma_1(^{2S+1}L_J)-\sigma_2(^{2S+1}L_J)\frac{1}{n}-\sigma_2^{\alpha}(^2P^0_{3/2},{}^1D_2)(n-m)\times(n-q)\sum_k \frac{1}{f_k(n,m,q,s)}\right\}^2. \quad (6)$$

The quantum defect is calculated from the standard formula

$$E_n = E_\infty - \frac{RZ^2}{(n-\delta)^2}. \quad (7)$$

2.2 Resonance energy and natural width of the the $1s^22s2p^6np\ {}^1P_1$ series

Using Eq. (5) we find (in Ryd)

$$\begin{aligned} E_n = E_\infty - \frac{1}{n^2}\Bigg\{Z-\sigma_1-\sigma_2\times\frac{1}{n}-\sigma_2\times(n-m)\times(n-q) \\ \times\left[\frac{1}{(n+q-m+s)^3}+\frac{1}{(n+q-m+s+1)^4}\right] \\ -\sigma_2\times(n-m)\times(n-q)^2\times\left[\frac{1}{(n+q+2s)^4}+\frac{1}{(n+m+s+1)^5}\right] \\ +\sigma_2^2\times(n-m)\times(n-q)^3\times\left[\frac{1}{(n+m+s)^5}+\frac{1}{(n+q-m+s)^6}\right]\Bigg\}^2. \end{aligned} \quad (8)$$

In addition, using (6), we express the natural width as follows (in Ryd)

$$\begin{aligned} \Gamma_n = \frac{1}{n^2}\Bigg\{Z-\sigma_1-\sigma_2\times\frac{1}{n}-\sigma_2\times(n-m)\times(n-q) \\ \times\left[\frac{1}{(n+q-m+s)^4}+\frac{1}{(n+q-m+s+1)^4}+\frac{1}{(n+q-m+1)^4}+\frac{1}{(n+q-m+s)^5}\right] \\ -\sigma_2\times(n-m)^2\times(n-q)\times\left[\frac{1}{(n+q-m+s+1)^5}+\frac{1}{(n+q-m+s)^6}\right]\Bigg\}^2. \end{aligned} \quad (9)$$

The σ_i-screening constants in Eqs. (8) and (4) are evaluated using Synchrotron radiation measurements of Schulz *et al.* [5].

2.3 Resonance energy of the $1s2s^22p^6np\ {}^1P_1$ series

In the same way, using Eqs. (5) we express the resonance energy of the $1s2s^22p^6np\ {}^1P_1$ series of Ne as follows (in Ryd)

$$\begin{aligned} E_n = I_K - \frac{1}{n^2}\Bigg\{Z-\sigma_1-\sigma_2\times\frac{1}{n}-\sigma_2^2\times(n-m)^2\times(n-q)\times\left[\frac{1}{(n+q-m+s)^4}+\frac{1}{(n+q-m)^5}\right] \\ -\sigma_2^2\times(n-m)\times(n-q)\times\left[\frac{1}{(n+q-m+s)^5}+\frac{1}{(n+m-q)^5}\right]\Bigg\}^2. \end{aligned} \quad (10)$$

The σ_i-screening constants in Eq. (10) are evaluated using Synchrotron radiation measurements of Müller *et al*. [7].

3. Results and Discussion

The results obtained in the present work are tabulated in Tables 1-4. Table 1 lists resonance energy of the $1s^2 2s2p^6 np$ $^1P_1$ series of Ne. Comparison of the present calculations from the *Modified atomic orbital theory* (MAOT) is done with other theoretical data from the *Screening constant by unit nuclear charge* (SCUNC) calculations of Sakho [6] and from the *Numerical calculations* (NC) of Schulz *et al*. [5] and with experimental data from *Synchrotron radiation* (SR) experiments of Schulz *et al*. [5] and from *Photoabsorption* (PA) experiments of Codling *et al*. [4]. The σ_i-screening constants in Eqs. (8) are evaluated using the experimental data of Schulz *et al*. [5] for the $1s^2 2s2p^6 3p$ $^1P_1$ ($m = 3$) and $1s^2 2s2p^6 4p$ $^1P_1$ ($q = 4$) levels equal to 45.5442 (50) eV and 47.1193 (50) eV, respectively. We get $\sigma_1 = 9.1265 \pm 0.0140$ and $\sigma_2 = -1.5567 \pm 0.0060$. In general, excellent agreements are obtained between theory and experiments.

Table 1. Resonance energy (E, eV) and effective quantum number n^* of the $1s^2 2s2p^6 np$ $^1P_1$ series of neutral Ne atom

	Theory			Experiments	
n	MAOT	SCUNC	NC	SR	PA
3	45.5441	45.5443	45.5340	45.5442 (50)	45.547 (9)
4	47.1192	47.1141	47.1109	47.1193 (50)	47.123 (6)
5	47.6943	47.6911	47.6918	47.6952 (15)	47.694 (6)
6	47.9670	47.9655	47.9671	47.9650 (30)	47.967 (6)
7	48.1177	48.1173	48.1186	48.1168 (20)	48.116 (6)
8	48.2099	48.2101	48.2111	48.2093 (20)	48.207 (6)
9	48.2705	48.2710	48.2717	48.2693 (20)	48.271 (6)
10	48.3125	48.3130	48.3136	48.3124 (10)	48.312 (6)
11	48.3428	48.3433	48.3437	48.3424 (10)	48.344 (6)
12	48.3654	48.3658	48.3662	48.3650 (10)	48.365 (6)
13	48.3827	48.3830	48.3833	48.3820 (10)	
14	48.3963	48.3964	48.3967	48.3954 (10)	
15	48.4071	48.4071	48.4073	48.4060 (10)	
16	48.4158	48.4158	48.4160	48.4147 (10)	
17	48.4230	48.4229	48.4230	48.4220 (10)	
18	48.4290	48.4288	48.4289	48.4280 (10)	
19	48.4340	48.4337	48.4338	48.4326 (10)	
20	48.4383	48.4379	48.4380	48.4370 (10)	

MAOT, Modified atomic orbital theory, present calculations
SCUNC, Screening constant by unit nuclear charge calculations of Sakho [6]
NC, Numerical calculations of Schulz *et al*. [5]
SR, Synchrotron radiation experiments of Schulz *et al*. [5]
PA, Photoabsorption experiments of Codling *et al*. [4]

Table 2 presents the effective quantum number $n^* = n-\delta$ of the doubly $1s^2 2s2p^6 np\ ^1P_1$ series of Ne. A shown in the work of Schulz *et al.* [5] for the $n > 7$ members exhibiting weak observable relativistic effects, the resonances are classified according to the relativistic jK coupling. Comparison shows that the MAOT results agree well with both the SCUNC calculations [6] and NC results [5] for $n < 10$. But for $n > 9$, the MAOT predictions are less precise. This is due to the simplicity of the formalism adopted in this work where the effective quantum number is given by $n^* = n-\delta$ in LS coupling, where δ is obtained from Eq. (7). Rigorously, due to strong electron correlation effects, the resonances analyzed in this work are best describe in jj coupling where the quantum defect $\delta_{nlj} = n - n^* + (j+1-[(j+1)^2 - (z\alpha)^2]^{1/2}$, where z is the asymptotic charge seen by the photoelectron and α is the fine-structure constant [13]. This may explain the behavior of the MOAT results regarding n^* for $n > 9$.

Table 2. Effective quantum number n^* of the $1s^2 2s2p^6 np\ ^1P_1$ series of neutral Ne atom

	Theory			Experiment
n	MAOT	SCUNC	NC	SR
3	2.15	2.15	2.15	2.155 (2)
4	3.17	3.16	3.16	3.168 (6)
5	4.17	4.17	4.17	4.177 (4)
6	5.18	5.17	5.18	5.17 (2)
7	6.17	6.17	6.18	6.16 (2)
8	7.16	7.17	7.18	7.16 (3)
9	8.16	8.17	8.18	8.13 (4)
10	9.15	9.16	9.18	9.15 (3)
11	10.14	10.16	10.18	10.13 (4)
12	11.14	11.16	11.18	11.12 (5)
13	12.14	12.16	12.18	12.10 (7)
14	13.14	13.16	13.18	13.07 (8)
15	14.15	14.16	14.18	14.04 (10)
16	15.16	15.16	15.18	15.02 (12)
17	16.18	16.16	16.18	16.02 (15)
18	17.20	17.16	17.18	17.01 (18)
19	18.22	18.16	18.18	17.91 (21)
20	19.25	19.15	19.18	18.92 (25)

SCUNC, Screening constant by unit nuclear charge calculations, present results
NC, Numerical calculations of Schulz *et al.* [10]
SR, Synchrotron radiation experiments of Schulz *et al.* [10]
PA, Photoabsorption experiments of Codling *et al.* [4]

Table 3 compares the present MAOT calculations of the width of the $1s^2 2s2p^6 np\ ^1P_1$ series of Ne with various theoretical and experimental literature data. The σ_i-screening constants in Eqs. (9) are evaluated using the experimental data of Colding *et al.* [4] for the $1s^2 2s2p^6 3p\ ^1P_1$ ($m = 3$) and $1s^2 2s2p^6 4p\ ^1P_1$ ($q = 4$) level respectively equal to 13 (2) meV and 4.5 (1.5) meV. We get then $\sigma_1 = 9.9872 \pm 0.0244$ and $\sigma_2 = -0.2398 \pm 0.0525$. In general good agreement is obtained between the quoted data. It should be underlined that, the present MAOT values for $n = 3$ and $n = 4$ match more with the calculations of Stener *et al.* [12], Nrisimhamurty *et al.* [13] and with the measurements of Codling *et al.* [4]. For $n > 4$, comparison shows excellent agreements with the SCUNC calculations [6] and the NC results [5] up to $n = 20$.

Table 3. Width (Γ, meV) of the $1s^22s2p^6np\ ^1P_1$ series of Ne

States	Theory							Experiment	
	Γ^M	Γ^S	Γ^a	Γ^b	Γ^c	Γ^d	Γ^e	$\Gamma^{a,b}$	Γ^f
3	13.00	13.08	34.9	18.6	11.4	13.9	13	16 (2)^a	13 (2)
4	4.50	4.53	6.65	4.3	5.28	3.86	7	5.7 (2)^b	4.5 (1.5)
5	2.05	1.98	2.47	1.8	2.61	1.62	3	3.6 (1.8)^b	2 (1)
6	1.10	1.04	1.28		1.44		1.58		
7	0.65	0.62	0.70						
8	0.42	0.40	0.46						
9	0.28	0.28	0.31						
10	0.20	0.20	0.22						
11	0.15	0.15	0.16						
12	0.11	0.12	0.12						
13	0.09	0.09	0.09						
14	0.07	0.08	0.07						
15	0.06	0.06	0.06						
16	0.04	0.05	0.05						
17	0.04	0.04	0.04						
18	0.03	0.04	0.03						
19	0.03	0.03	0.03						
20	0.02	0.03	0.02						

m, Modified atomic orbital theory, present calculations
s, Screening constant by unit nuclear charge calculations of Sakho [6]
a, Schulz *et al.* [5]
b, Langer *et al.* [10]
c, Liang *et al.* [11]
d, Stener *et al.* [12]
e, Nrisimhamurty *et al.* [13]
f, Codling *et al.* [4]

Table 4 presents resonance energy of the $1s2s^22p^6np\ ^1P_1$ series of neutral Ne atom. Comparison of the present calculations is done with various literature data [7, 14–21] as quoted in the work of Müller *et al.* [7]. For these states, the σ_i-screening constants in Eqs. (10) are evaluated using the experimental data of Müller *et al.* [7] for the $1s^22s2p^63p\ ^1P_1$ $(m = 3)$ and $1s^22s2p^64p\ ^1P_1$ $(q = 4)$ level respectively equal to 867.290 eV and 868.928 eV. For the binding energy I_K in neutral Ne atom we use the value suggested by NIST, $I_K = 870.23 \pm 0.18$ eV [22, 23]. We get then $\sigma_1 = 9.234 \pm 0.205$ and $\sigma_2 = -1.886 \pm 0.488$. Comparison indicates very good agreement between the MOAT calculations and the quoted literature data up to $n = 6$. The very good agreement between the MOAT predictions and the recent synchrotron measurement of Müller *et al*. [7] allows one to expect the MAOT quoted resonance energies for n = 7-20 as accurate.

Table 4. Resonance energies (E, eV) of the $1s2s^22p^6np\ ^1P_1$ series of Ne. The resonance are obtained from the state of Ne

	E^p	E^a	E^b	E^c	E^d	E^e	E^f	E^g	E^h	E^h
3	867.290	867.290	867.25	867.18	867.12	867.05	867.25	867.13	867.13	867.12
4	868.928	868.928	868.90	868.85	868.75	868.68	868.84	868.65	868.76	868.69
5	869.540	869.530	869.50	869.47	869.32	869.23	869.50	869.36	869.36	869.27
6	869.814	869.815	869.78	869.75	869.60	869.63				
7	869.957									
8	870.039									
9	870.090									
10	870.123									
11	870.146									
12	870.162									
13	870.174									
14	870.183									
15	870.190									
16	870.196									
17	870.200									
18	870.204									
19	870.207									
20	870.209									

p, present calculations
a, Müller *et al*. [7]
b, Wuilleumier, uncorrected [14]
c, Teodorescu *et al*. [15]
d, Saitoh *et al*. [16]
e, Hitchcock and Brion [17]
f, Esteva *et al*. [18]
g, Avaldi *et al*. [19]
h, Kato *et al*. [20]
i, Coreno *et al*. [21]

4. Conclusion

The *Modified Atomic Orbital Theory* (MAOT) has been applied to the Photoionization of Ne neutral atom. Accurate resonance energy and natural width of the $1s2s^22p^6np\ ^1P^1$ and $1s^22s2p^6np\ ^1P_1$ series of Ne. Overall, the present MAOT calculations agree very well with various literature data. The high lying accurate resonance energies tabulated may be benchmarked data for interpreting spectra lines from Ne neutral atom in astrophysical objects. The results obtained in this work may also be useful data for the NIST database.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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