

Spectroscopic Study of the Doubly Excited $^1G^e$ and $^3G^e$ Even States of the $Z = 8$ Heliumoid System Converging to the $N = 3$ Threshold of the Residual Ion

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To cite this article:

Oumar Ndiaye, Nogaye Ndiaye, Oumar Tidiane Ba, Djicknack Dione, Papa Macoumba Faye et al. (2025). Spectroscopic Study of the Doubly Excited $^1G^e$ and $^3G^e$ Even States of the $Z = 8$ Heliumoid System Converging to the $N = 3$ Threshold of the Residual Ion. *American Journal of Modern Physics*, 14(2), 52-59. <https://doi.org/10.11648/j.ajmp.20251402.12>

Received: 6 May 2024; **Accepted:** 27 May 2024; **Published:** 31 March 2025

Abstract: Doubly excited systems, particularly in heliumoid configurations, represent a complex area of research due to the strong interactions between the electrons. The diagonalization method is a powerful technique for studying these systems, simplifying the problem to a system of linear algebraic equations. This method makes it possible to obtain resonance parameters, such as energies E and partial widths Γ , with great precision. In the literature, there are no experimental measurements of the energies of doubly excited states in heliumoid systems, nor of the associated partial widths. The theoretical results available are few and often show inconsistencies. Moreover, even states have not yet been treated exhaustively using diagonalization or other theoretical methods. In this work, we focus on doubly excited resonances of $^{1,3}G^e$ symmetry sublevels. Using a diagonalization method, we have performed robust numerical calculations to determine the resonance parameters (energies E and widths Γ) of the $(3l_1kl_2)^{1,3}G^e$ states of the ion. The numerical advantages of the diagonalization method make it possible to obtain these resonance parameters simply and accurately. We report for the first time the resonance parameters of the $^{1,3}G^e$ states, including E energies and Γ partial widths. The calculations have shown high accuracy, with results consistent with the few existing theoretical data. This study makes a significant contribution to our understanding of doubly excited states in heliumoid systems. These results fill a gap in the literature and provide a solid basis for future theoretical and experimental studies. The numerical advantages of the diagonalization method make it a technique of choice for the study of complex quantum systems. The results obtained pave the way for further investigations into other configurations and symmetries of doubly excited states. They also encourage the development of experimental measurements to validate theoretical predictions and improve our understanding of self-ionization processes in multi-electron ions.

Keywords: O^{6+} He-type, Doubly Excited States, Electronic Correlation, Diagonalization Method, $^{1,3}G^e$ Resonance Series

1. Introduction

As mentioned in a previous paper in Atomic Physics [1], the discovery of the strong electron-electron correlation in the double-excited states of helium during the Madden and Codling experiments [2], sparked sustained interest in the study of He-type autoionization states and their properties [3, 4]. Many resonances in the helium absorption spectrum

have since been observed. Considerable progress has thus been made in the study of the autoionization states of two-electron systems. This is ensured by atomic and ionic spectroscopy techniques of increasingly intense photon sources by synchrotron radiation. In addition, autoionization states in the electromagnetic spectrum, which are found in very extended domains, are being studied, particularly in the

context of plasma states [5]. We should also mention that these double-excited electron states are observed in atomic collision experiments, which lead to electron capture. There have been a series of experimental studies on electron transfer collisions between a strongly empty ion and a neutral atom. We are interested in such experiments as the formation of double-excited autoionization states of O^{6+} ions below the $N = 4$ thresholds of odd states and the $N = 3$ thresholds in collisions of O^{8+} ions on He atoms [6, 7]. We require knowledge of a large range of data, i.e. an oxygen ion production databank, and even an understanding of odd and even autoionization states. In the literature, we have seen many calculations, for example on resonance positions over the Helium atom ($Z \leq 2$). Most of these positions, in the case of very large Z , are determined by theoretical approaches [8, 9]. However, in the exceptional case of the helium atom, these resonance positions are calculated using a various approaches. Among these methods are the saddle-point complex-rotation method [10, 11], the close-coupling method [12], the truncated-diagonalization method [13], the discretization technique [14, 15], the complex coordinate rotation [16, 17], the computing double sum over the complete hydrogen spectrum [18], the density functional theory [19], the Feshbach-projection formalism [20], the spin-dependent localized Hartree-Fock density-functional method [21], the method combining Hylleraas and incomplete hydrogenic wave functions [22] and semi-empirical method [23]. For most of the preceding methods, calculations are performed mainly for resonance energies and total widths. The extension of these methods to the calculation of partial widths, which is, the probabilities of decay into various exit channels, is less well established. The diagonalization method is used in this investigation (see Ref. [24]). This method is adopted here, as it provides a means of determining resonance positions, partial widths and total widths. The diagonalization approximation assumes the coupling of closed and open channels as the perturbation term in the hamiltonien system and neglects the indirect coupling of autoionization states through open channels. This procedure will eventually leads to a mathematical concept based on a set of relatively simple problems. This means a system of linear algebraic equations instead of a system of coupled differential equations or integro-differential equations [25, 26]. The use of this diagonalization method has been very fruitful for calculations of the $L=1$ resonance states of two-electron atoms. It has also been used extensively to calculate the partial widths of triplet and singlet resonance odd states $^{1,3}L^o$ symmetry for L ranging from 1 to 7. This paper deals with the study of the partial widths of the multi-channel decay of the even states denoted $^{1,3}G^e$ of the heliumoid system at $Z = 8$ converging to the threshold $N = 3$ of the residual O^{6+} ion. It will be organized as follows: in section 1, a general introduction to two-electron systems is given. Then, in section 2, the theoretical basis and details of the method for solving the physical hamiltonian defined in this work are explained; followed by section 3 reserved for results and discussion, and finally a conclusion in section 4.

2. Theory and Methods

For an effective description of the excitation and de-excitation processes of autoionization states, it is necessary to use computational techniques that take into account the mixing of configurations as much as possible. The diagonalization method, which is a simplification of the Fano method [27], is one such computational technique. It has been successfully applied to the study of single-channel resonant photoionization (interaction of one or more resonances with a single continuum) of some two-electron systems below the residual ion threshold $N = 2$ [28]. This method was then generalized to the study of multi-channel resonant photoionization (interaction of one or more resonances with several continua) for the description of the $(3s3p)^1P^o$ resonance of helium [29] and in the study of multicharged heliumoid systems under residual ion thresholds $N = 2$ and $N = 3$ [30]. In its practical application, the diagonalization method involves solving systems of algebraic equations to obtain the wave functions and energies of the autoionizing states, and then determining the partial and total widths, as well as the effective photoionization cross-section. The wave function $\Psi_{E_i}(\mathbf{r}_1, \mathbf{r}_2)$ represents the solution of the following Schrödinger equation:

$$\hat{H}\Psi_E(\mathbf{r}_1, \mathbf{r}_2) = E\Psi_E(\mathbf{r}_1, \mathbf{r}_2) \quad (1)$$

with

$$\hat{H} = \hat{H}_0 + \hat{V}, \quad (2)$$

\hat{H}_0 being the zero-order hamiltonian and \hat{V} the coulomb interaction operator between the two-electrons, is decomposed as in Fano's method [27] into two parts: one containing the subspace of open channels (discrete states) and another comprising the subspace of closed channels (continua states). This function is therefore expressed as follows:

$$\begin{aligned} \Psi_E(\mathbf{r}_1, \mathbf{r}_2) = & \sum_k \hat{A} [\psi_k(\mathbf{r}_1) U_k(E, \mathbf{r}_2)] \\ & + \sum_{\mu} \Lambda_{\mu} \phi_{\mu}(\mathbf{r}_1, \mathbf{r}_2). \end{aligned} \quad (3)$$

In this equation, k designates the set of quantum numbers characterizing the system formed by the residual ion and the electron ejected below the open channels. Also in this equation, the summation over μ is centered only at doubly excited states. \hat{A} , represents the antisymmetrization operator and $U_k(E, \mathbf{r}_2)$ is an unknown wave function to be determined. In fact, this wave function describes the behavior of the electron ejected from the system while the residual ion is described by the wave function $\psi_k(\mathbf{r}_1)$. The Λ_{μ} are coefficients to be determined likewise. The wave function describing the residual ion must satisfy the following conditions:

$$\langle \psi_k(\mathbf{r}) | \psi_{k'}(\mathbf{r}) \rangle = \delta_{k,k'} \quad (4)$$

$$\langle \psi_k(\mathbf{r}) | \hat{H} | \psi_{k'}(\mathbf{r}) \rangle = \epsilon_{k,k'} \delta_{k,k'} + \hat{V}_{k,k'} \quad (5)$$

In equation (4), $\hat{V}_{k,k'}$ designates the matrix element of the coulombian interaction operator via two-electrons. However, also in equation (3), the wave function describing the autoionization states is given by $\phi_\mu(\mathbf{r}_1, \mathbf{r}_2)$. This function is

obtained by unitary transformation of the (\hat{H} hamiltonian of the system in the subspace of closed channels. It comes to be described by :

$$\phi_\mu(\mathbf{r}_1, \mathbf{r}_2) = \sum_{j,l} \alpha_\mu(j, l) \hat{A} [\psi_j(\mathbf{r}) \psi_l(\mathbf{r})]. \quad (6)$$

These wave functions satisfy the following condition:

$$\langle \psi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \hat{H} | \psi_{\mu'}(\mathbf{r}_1, \mathbf{r}_2) \rangle = \epsilon_{\mu,\mu'} \delta_{\mu,\mu'}. \quad (7)$$

The coefficient $\alpha_\mu(j, l)$ in equation (6) is obtained by solving the following algebraic system:

$$\sum_{\nu} \{ (E - E_0) \delta_{\mu,\mu'} + \langle \chi_\mu | \hat{V} | \chi_{\mu'} \rangle \} \alpha_\nu = 0. \quad (8)$$

In this algebraic system, the E_0 represents the eigenvalue of the hamiltonian \hat{H}_0 corresponding to the χ_μ eigenfunctions. The introduction of a total wave function into the Schrödinger equation and some operators give us to find the Λ_μ and $U_k(E, \mathbf{r}_2)$ [31]. Solving the system of equation (9) and equation (10) provides the expression of the wave function of the final state of the ejected electron.

$$\begin{aligned} \Lambda_\mu(E) = & \frac{\sum_{j=0}^N \langle \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \hat{V} | \hat{A} [U_j(E, \mathbf{r}_2) \psi_j(\mathbf{r}_1)] \rangle}{E - \epsilon_\mu} \times \left[-\frac{1}{2} \nabla^2 - \frac{Z}{\mathbf{r}_2} + \langle \psi_j(\mathbf{r}_1) | \hat{V} | \psi_j(\mathbf{r}_2) \rangle \right] U_j(E, \mathbf{r}_2) \\ & \times (E_j - E) U_j(E, \mathbf{r}_2) \pm \langle \psi_j(\mathbf{r}_1) | \hat{V} | U_j(E, \mathbf{r}_1) \psi_j(\mathbf{r}_2) \rangle \end{aligned} \quad (9)$$

and

$$\sum_{k \neq j} \langle \psi_j(\mathbf{r}_1) | \hat{V} | X_j \rangle = \sqrt{2} \sum_{\mu} \Lambda_\mu(E) Y_j^\mu \quad (10)$$

with $X_j = \hat{A} [U_j(E, \mathbf{r}_1) \psi_j(\mathbf{r}_2)]$ and $Y_j^\mu = \langle \psi_j(\mathbf{r}_1) | \hat{V} | \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) \rangle$. This final state of the ejected electron is defined as follows in equation (11):

$$\begin{aligned} \Psi_E(\mathbf{r}_1, \mathbf{r}_2) = & \varphi_j(E) + \frac{\langle \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \hat{V} | \varphi_j(E) \rangle}{E - \epsilon_\mu - \Delta_\mu - \frac{i}{2} \Gamma_\mu^{\text{tot}}} \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) \\ & + i\pi \frac{\langle \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \hat{V} | \varphi_j(E) \rangle}{E - \epsilon_\mu - \Delta_\mu - \frac{i}{2} \Gamma_\mu^{\text{tot}}} \sum_i \varphi_i(E) \times \langle \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \hat{V} | \varphi_j(E) \rangle \end{aligned} \quad (11)$$

In this equation (11), the wave function $\varphi_j(E)$ describes the continuum spectrum with electrostatic coupling of the first order in the open channel.

This wave function is defined as follows:

$$\varphi_j(E) = \hat{A} [\delta_{k,j} \Psi_j(E, \mathbf{r}_2) \Psi_k(\mathbf{r}_1)] \quad (12)$$

In these equations, Γ_μ^{tot} is the total width of the autoionization state and is obtained by:

$$\Gamma_\mu^{\text{tot}} = 2\pi \sum_j |\langle \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \hat{V} | \varphi_j(E) \rangle|^2. \quad (13)$$

This leads to the mathematical definition of the partial width Γ_μ^μ as follow :

$$\Gamma_j^\mu = 2\pi |\langle \phi_\mu(\mathbf{r}_1, \mathbf{r}_2) | \frac{1}{\mathbf{r}_{12}} | \varphi_j(E) \rangle|^2 \text{ with } \Gamma^{\text{tot}} = \sum_j \Gamma_j^\mu \quad (14)$$

3. Results and Discussion

In this study, all interest is focused on the question of partial widths shown in (14) of even singlets and triplets defined by $(3l_1kl_2)^{1,3}G^e$. It has been carried out by applying the method of diagonalization of the hamiltonian matrices according to some postulates derived from quantum physics. The physical system considered in this work is that of a heliumoid at $Z = 8$ converging to the $N = 3$ threshold of excitation. As such, they have the only possibility of decaying into four open channels 1skg, 2skg, 2pkf and 2pkh in the case of $^1G^e$ and 2pkf and 2pkh in the latter case of $^3G^e$. In this description, we could have simply taken the notation of these open channels of the $^{1,3}G^e$ respectively as follows: 10k4, 20k4, 21k3 and 21k5. This gives in the sense, two interesting items of information in Russel-Sanders notation $^{1,3}L^\pi$: (i) the sum of the second character and the last character gives the value of L with ($L = l_1 + l_2$); (ii) as this sum is even, it indicates the π parity of the state, which is even here. According to the notion of $(3l_1kl_2)$, the first two characters indicate the state of the residual ion, while the last two communicate the wave number of the ejected electron and its angular momentum. The calculation of partial decay widths according to the diagonalization approximation, taking into account the coupling of open and closed channels, has enabled us to obtain results. We have divided our results into two sub-sections in order to do a comparative analysis between singlet and triplet states.

3.1. Even Singlet States

This subsection is focused on the $(3l_1kl_2)^1G^e$ singlet symmetry states. Calculations are based on the 48 decay sublevels of the $^1G^e$ state using the diagonalization method applied to the O^{6+} state under the $N = 3$ threshold. In table 1, the resonance widths are listed for various doubly excited states of the oxygen ion O^{6+} , in particular the 3d5d and 3d6f states. These states do not decay below the ionization threshold $N = 3$. This means that, for these states, the resonance energy is lower than the energy required to ionize the ion and release an electron. However, decay in open channels is theoretically predictable. This prediction is based on in-depth theoretical calculations that take into account the complex interactions between electrons and possible de-excitation processes. Indeed, although these states are bound, they can decay by releasing an electron if enough energy is supplied to overcome the ionization threshold. All the states listed in Table 1 decay in the four open channels 1skg, 2skg, 2pkf and 2pkh, with the exception of the 3d6f and 3p6f states. However, the 3d5d \rightarrow 1skg and 3d6f \rightarrow 1skg states exhibit a resonance width $\Gamma = 0.00000$ ev, indicating that they do not decay in this specific channel.

The decay channels mentioned (1skg, 2skg, 2pkf and 2pkh) are essential for understanding the decay mechanisms of doubly excited states. The Γ resonance widths indicate the probability of decay through these previously mentioned channels.

Table 1. Partial widths Γ_{3dkl_2} (in ev) of the $^1G^e$ autoionization states of the O^{6+} ion converging to the $N = 3$ threshold of O^{7+} .

| States | Γ (ev) |
|-------------------------|---------------|
| 3d3d \rightarrow 1skg | 0.00000049 |
| 3d3d \rightarrow 2skg | 0.00031853 |
| 3d3d \rightarrow 2pkf | 0.00004190 |
| 3d3d \rightarrow 2pkh | 0.00007014 |
| 3d4d \rightarrow 1skg | 0.000000080 |
| 3d4d \rightarrow 2skg | 0.00000098 |
| 3d4d \rightarrow 2pkf | 0.00000195 |
| 3d4d \rightarrow 2pkh | 0.00000959 |
| 3d5d \rightarrow 1skg | 0.00000000 |
| 3d5d \rightarrow 2skg | 0.00001308 |
| 3d5d \rightarrow 2pkf | 0.00020558 |
| 3d5d \rightarrow 2pkh | 0.00006712 |
| 3d6d \rightarrow 1skg | 0.00000043 |
| 3d6d \rightarrow 2skg | 0.0000935 |
| 3d6d \rightarrow 2pkf | 0.00003565 |
| 3d6d \rightarrow 2pkh | 0.00001825 |
| 3d5g \rightarrow 1skg | 0.00000052 |
| 3d5g \rightarrow 2skg | 0.00014057 |
| 3d5g \rightarrow 2pkf | 0.00002013 |
| 3d5g \rightarrow 2pkh | 0.00003186 |
| 3d6g \rightarrow 1skg | 0.00000010 |
| 3d6g \rightarrow 2skg | 0.00000192 |
| 3d6g \rightarrow 2pkf | 0.00039533 |
| 3d6g \rightarrow 2pkh | 0.00002125 |
| 3d6f \rightarrow 1skg | 0.00000000 |
| 3d6f \rightarrow 2skg | 0.00003166 |

Table 2. Partial widths Γ_{3pkl_2} (in eV) of the $^1G^e$ autoionization states of the O^{6+} ion converging to the $N = 3$ threshold of O^{7+} .

| States | Γ (ev) |
|-------------------------|---------------|
| 3p4f \rightarrow 1skg | 0.00000142 |
| 3p4f \rightarrow 2skg | 0.00051194 |
| 3p4f \rightarrow 2pkf | 0.00008007 |
| 3p4f \rightarrow 2pkh | 0.00008275 |
| 3p5f \rightarrow 1skg | 0.000000030 |
| 3p5f \rightarrow 2skg | 0.000000060 |
| 3p5f \rightarrow 2pkf | 0.00000437 |
| 3p5f \rightarrow 2pkh | 0.00001602 |
| 3p6f \rightarrow 2pkf | 0.000741 |
| 3p6f \rightarrow 2pkh | 0.00006852 |
| 3p6h \rightarrow 1skg | 0.00000000 |
| 3p6h \rightarrow 2skg | 0.00000000 |
| 3p6h \rightarrow 2pkf | 0.00000000 |
| 3p6h \rightarrow 2pkh | 0.00000000 |

Table 2 clearly shows the partial width results for the 3p4f, 3p5f, 3p6f and 3p6h states in the 1skg, 2skg, 2pkf and 2pkh open channels. The results highlight several key points concerning the decay of 3pkl2 states ($l_2 = 3, 5$) in open channels. In (i), the 3p6f states show a strong tendency to decay in the 2pkf channel. This is revealed by a significantly

larger resonance width for this channel compared with the other open channels. This tendency may be due to factors such as coupling interactions between electrons and the energy levels available in this specific channel. And in (ii), the 3p6h states show strongly restricted decay in the open channels. The Γ resonance widths for these states are significantly smaller in all channels, indicating a lower decay probability. This restriction can be attributed to structural or energetic reasons specific to these states.

Table 3 shows the results of calculations of the partial decay widths of the 3s5g and 3s6g sublevels of the O^{6+} system in the open channels 1skg, 2skg, 2pkf and 2pkh. As opposed to the 3d and 3p sublevels, the 3s sublevels of the G states show no tendency towards restricted decay. This means that all 3s5g and 3s6g sublevels have fully decayed below the specified open channels. The partial width values for the 3s5g and 3s6g sublevels show a predominance of the 2pkf channel, particularly when the system is in the 3s6g sublevel. This suggests that the 2pkf channel is the preferred decay path for these states.

Table 3. Partial widths Γ_{3skl} (in eV) of the $^1G^e$ autoionization states of the O^{6+} ion converging to the $N = 3$ threshold of O^{7+}

| States | Γ (ev) |
|-------------------------|---------------|
| 3s5g \rightarrow 1skg | 0.00000052 |
| 3s5g \rightarrow 2skg | 0.00014070 |
| 3s5g \rightarrow 2pkf | 0.00002012 |
| 3s5g \rightarrow 2pkh | 0.00003185 |
| 3s6g \rightarrow 1skg | 0.000000010 |
| 3s6g \rightarrow 2skg | 0.00000191 |
| 3s6g \rightarrow 2pkf | 0.00039539 |
| 3s6g \rightarrow 2pkh | 0.00002127 |

In conclusion, the study of the $^1G^e$ singlet states of the O^{6+} physical system that decay below the threshold of $N = 3$ to the residual ion O^{7+} according to the application of diagonalization has helped us to compare the values of the partial widths. The application of this method showed that there are restricted decays below the $N = 3$ threshold. It also demonstrated the variability of partial widths, which competed in a predominance. This suggests a strong decay preference of the system towards a given open channel. Thus, the partial widths of the 3d, 3p and 3s dominants are respectively $\Gamma_{3dkl} = 0.0003953$, $\Gamma_{3pkl} = 0.000741$ and $\Gamma_{3skl} = 0.00039539$. These are the respective decays of 3d6g \rightarrow 2pkf, 3p6f \rightarrow 2pkf and 3s6g \rightarrow 2pkf.

3.2. Even Triplet States

In the general Russel-Sanders notation, triplet states $^{2S+1}L\pi$ are characterized by $S = 1$ in which S is as the sum of the spins of the particles (here electrons): $S = s_1 + s_2$ with s_i ($i = 1, 2$), the electron's spin value. However, in quantum mechanics, triplets states describe, for example, the state of two 1/2-spin particles. This is why, in this subsection, we focus on the triplet states of the two-electron O^{6+} system. All decay below

the threshold of $N = 3$ into the residual ion O^{7+} . Applying the diagonalization approximation to study the multichannel decay of the $^3G^e$ triplet state yielded 24 sub-levels $3l_1k l_2$ $^3G^e$. This led to the partial decay widths of O^{6+} below the threshold of $N = 3$ into O^{7+} .

Table 4. Partial widths Γ_{3dkl} (in eV) of the $^3G^e$ autoionization states of the O^{6+} ion converging to the $N = 3$ threshold of O^{7+}

| States | Γ (ev) |
|-------------------------|---------------|
| 3d3d \rightarrow 2pkf | 0.00003687 |
| 3d3d \rightarrow 2pkh | 0.00006778 |
| 3d4d \rightarrow 2pkf | 0.00016257 |
| 3d4d \rightarrow 2pkh | 0.00014899 |
| 3d5d \rightarrow 2pkf | 0.00000081 |
| 3d5d \rightarrow 2pkh | 0.00000022 |
| 3d6d \rightarrow 2pkf | 0.00007109 |
| 3d6d \rightarrow 2pkh | 0.00002227 |
| 3d5g \rightarrow 2pkf | 0.00039121 |
| 3d5g \rightarrow 2pkh | 0.0000198 |
| 3d6g \rightarrow 2pkf | 0.00029847 |
| 3d6g \rightarrow 2pkh | 0.00008296 |

Among the 24 sublevels of triplet states, the table 4 focused specifically on sublevels 3d3d, 3d4d, 3d5d, 3d6d, 3d5g and 3d6g. All these sublevels decay towards the open channels 2pkf and 2pkh. The results show a marked preference for decay in the 2pkf channel. This trend is particularly pronounced for the 3d5g sublevel, with a partial decay width $\Gamma_{3dkl \rightarrow 2pkf} = 0.00039121$.

Table 5. Partial widths Γ_{3pkl} (in eV) of the $^3G^e$ autoionization states of the O^{6+} ion converging to the $N = 3$ threshold of O^{7+}

| States | Γ (ev) |
|-------------------------|---------------|
| 3p4f \rightarrow 2pkf | 0.00042297 |
| 3p4f \rightarrow 2pkh | 0.00009622 |
| 3p5f \rightarrow 2pkf | 0.00007631 |
| 3p5f \rightarrow 2pkh | 0.00001973 |
| 3p6f \rightarrow 2pkf | 0.00078808 |
| 3p6f \rightarrow 2pkh | 0.00000053 |
| 3p6h \rightarrow 2pkf | 0.00000000 |
| 3p6h \rightarrow 2pkh | 0.00000000 |

Table 5 shows the partial widths of the 3p sublevels of O^{6+} . It is important to note two specific restricted decays: $\Gamma_{3p6h \rightarrow 2pkf} = 0.0000000$ eV and $\Gamma_{3p6h \rightarrow 2pkh} = 0.0000000$ eV. These values indicate that the 3p6h sublevel does not decay through the 2pkf and 2pkh channels below the $N = 3$ threshold of the residual O^{7+} ion. This observation reveals an immediate difference in stability between the 3d and 3p sublevels of O^{6+} . Moreover, the most significant partial width observed is: $\Gamma_{3pkl} = 0.00078808$ eV. This value far exceeds those noted for the 3d sublevels. This indicates that, in some cases, 3p sublevels can show more pronounced decays than 3d sublevels.

Table 6. Partial widths Γ_{3skl} (in eV) of the $^3G^e$ autoionization states of the O^{6+} ion converging to the $N = 3$ threshold of O^{7+}

| States | Γ (ev) |
|-------------------------|---------------|
| $3s5g \rightarrow 2pkf$ | 0.00039121 |
| $3s5g \rightarrow 2pkh$ | 0.00001988 |
| $3s6g \rightarrow 2pkf$ | 0.00029850 |
| $3s6g \rightarrow 2pkh$ | 0.00008297 |

Table 6 shows the partial widths of the 3s sublevels of O^{6+} . The analysis shows that all four 3s sublevels decay below

the open channels 2pkf and 2pkh. It is important to note a marked preference for decay towards the 2pkf channel, with a significant partial width: $\Gamma_{3skl \rightarrow 2pkf} = 0.00039121$ eV. This value indicates that, among the open channels available, the 2pkf channel is favored for 3s sublevel decay.

The study of the $^3G^e$ singlet states of the physical system O^{6+} , which decay below the threshold of $N = 3$ to the residual ion O^{7+} , was carried out using the diagonalization method. This approach enabled us to compare the values of the partial widths of the different sublevels. In (i): the 3d, 3p and 3s sublevels decay mainly into the 2pkf and 2pkh open channels.

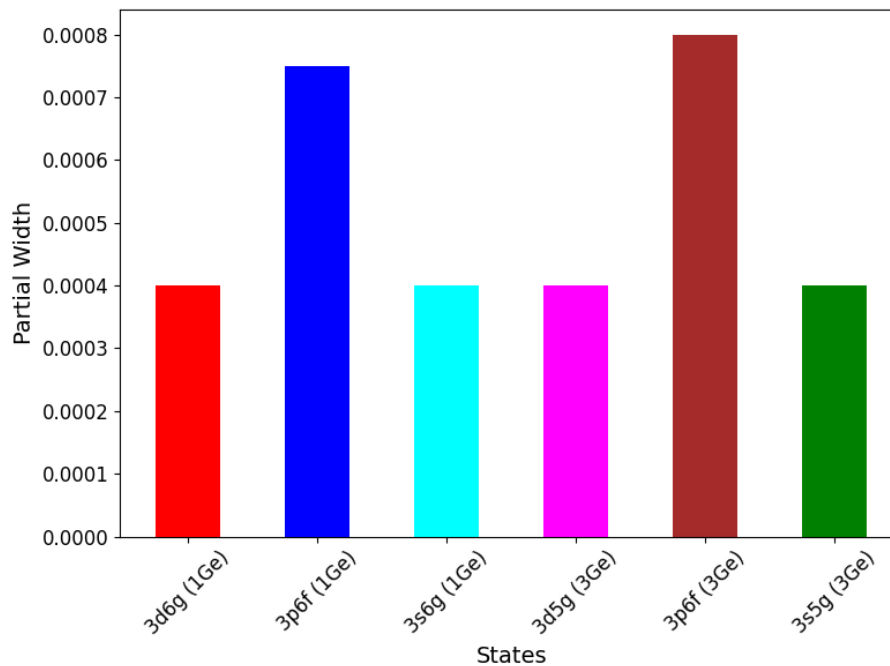


Figure 1. Competition of partial widths Γ (in eV) of the $^{1,3}G^e$. In red bands, we compare the decaying from states 3d6g, 3s6g sub-levels of $^1G^e$ and the 3d5g, 3s5g sub-levels of $^3G^e$ to the 2pkf open channel; respectively, in blue and green band, we mention the decaying from states 3p6f($^1G^e$) and 3p6f($^3G^e$) to the 2pkf open channel.

A significant preference was observed for decay towards the 2pkf channel, with significant partial widths, particularly for the 3d5g and 3s sublevels, where $\Gamma_{3skl \rightarrow 2pkf} = 0.00039121$ eV (see in Table 4. In (ii): The 3p6h sublevels show restricted decays, not decaying through the 2pkf and 2pkh channels below the $N = 3$ threshold of the residual ion O^{7+} , indicating a notable difference in stability compared to the other 3d and 3p sublevels. And finally in (iii), the most relevant partial width observed for the 3p sublevels is $\Gamma_{3pkl \rightarrow 2pkf} = 0.00078808$ eV (see in Table 5, surpassing the values noted for the 3d sublevels.

For instance, in Figure 1, bar diagrams show the dominant partial widths in the decay process of the O^{6+} system. These diagrams illustrate the competition between the 3d6g and 3s6g sublevels of $^1G^e$ and the 3d5g and 3s5g sublevels of $^3G^e$. Blue bars, representing the singlet state ($^1G^e$), and green bars, representing the triplet state ($^3G^e$), indicate the dominance of the 3p6f sublevel during the decay process. The results suggest that decay of O^{6+} below the $N = 3$ threshold of the O^{7+} ion

occurs mainly through the 2pkf open channels arising from the 3p6f sublevels, in both the singlet and triplet states.

4. Conclusion

The diagonalization calculations reported in this paper produced excitation energies and partial widths in agreement with those obtained by other works cited, using other theoretical methods. However, when the direct coupling between the open channels is neglected, some differences appear. Although this approximation is reasonable for systems with a high nuclear charge, a more detailed analysis is required. The results reveal competition between the 3d6g and 3s6g sublevels of $^1G^e$, as well as the 3d5g and 3s5g sublevels of $^3G^e$, in the decay of the O^{6+} system. The partial width values of $^1G^e$ and $^3G^e$ reveal the predominance of the 3p6f sublevel during decay. Furthermore, they indicate that the decay of O^{6+} below the $N = 3$ threshold of the O^{7+} ion

occurs mainly in the 2pkf open channels, originating from the 3p6f sublevels, in both singlet and triplet states. These remarkable results, particularly significant for even states, have never been explored in atomic physics. So, in the near future, we plan to carry out calculations using pure quantum qubits, offering a better understanding of particle dynamics under similar conditions.

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Acknowledgments

We gratefully acknowledge conversations with Professor Ababacar Sadikhe Ndao.

Computer were provided by the Institute of Applied Nuclear Technology (IANT), University Cheikh Anta Diop, Dakar-Fann, Senegal.

Conflicts of Interest

The authors declare no conflicts of interest.

References

- [1] Oumar Ndiaye, Oumar Tidiane Ba, Papa Macoumba Faye, Nogaye Ndiaye, Djicknack Dione, Jean Paul Latyr Faye, Alassane Traore, Ababacar Sadikhe Ndao. Multi-channel Decay Partial Widths of $^{1,3}L^o$ Auto-ionizing Levels of O^{6+} below $N=5$ Threshold. Nuclear Science. Vol. 6, No. 4, 2021, pp. 26-34. <https://doi.org/10.11648/j.ns.20210604.11>
- [2] Madden, R. P., & Codling, K. (1965). Two-Electron Excitation States in Helium. The Astrophysical Journal, 141, 364. <https://doi.org/10.1086/148132>
- [3] Codling, K., Madden, R. P., & Ederer, D. L. (1967). Resonances in the photo-ionization continuum of Ne I (20-150eV). Physical Review, 155(1), 26. <https://doi.org/10.1103/PhysRev.155.26>
- [4] Madden, R. P., Ederer, D. L., & Codling, K. (1969). Resonances in the photo-ionization continuum of Ar I (20-150 eV). Physical Review, 177(1), 136. <https://doi.org/10.1103/PhysRev.177.136>
- [5] Liang, L., Gao, W., Zhou, C., & Zhang, L. (2012). Calculation of fine-structure energy levels and autoionizing widths for the magnesium-like ions Ti XI and Fe XV. Atomic Data and Nuclear Data Tables, 98(1), 63-73. <https://doi.org/10.1016/j.adt.2011.08.003>
- [6] Wu, Y., et al. "Theoretical investigation of total and state-dependent charge exchange in O^{6+} collisions with atomic hydrogen." Journal of Physics B: Atomic, Molecular and Optical Physics 45.23 (2012): 235201. <https://doi.org/10.1088/0953-4075/45/23/235201>
- [7] Nahar, Sultana N. "Photoionization of Ar XVI and Ar XVII." Journal of Quantitative Spectroscopy and Radiative Transfer 117 (2013): 15-20. <https://doi.org/10.1016/j.jqsrt.2012.12.001>
- [8] Johnson, W. R., et al. "E1 transitions between states with $n=1-6$ in helium-like carbon, nitrogen, oxygen, neon, silicon, and argon." The Astrophysical Journal Supplement Series 141.2 (2002): 543. <https://doi.org/10.1086/340547>
- [9] Diallo, Abdourahmane, et al. "Variational Calculation of the Doubly-Excited States N_{snp} of He-Like Ions via the Modified Atomic Orbitals Theory." Journal of Modern Physics 12.02 (2021): 105. <https://doi.org/10.4236/jmp.2021.122011>
- [10] Moretto-Capelle, P., et al. "Double capture in the O^{8++} He collision investigated by electron spectroscopy (80 keV, $10'$)." Journal of Physics B: Atomic, Molecular and Optical Physics 22.2 (1989): 271. <https://doi.org/10.1088/0953-4075/22/2/015>
- [11] Bliman, S., et al. "Charge exchange in the O^{8+} -He collision at keV amu^{-1} energies." Journal of Physics B: Atomic and Molecular Physics 16.15 (1983): 2849. <https://doi.org/10.1088/0022-3700/16/15/025>
- [12] Chen, Ming-Keh. "Doubly excited $^{1,3}S^e, ^{1,3}P^o$, and $^{1,3}D$ resonances in He below the $N = 2$ He^+ threshold." PHYSICAL REVIEW A 56.6 (1997): 4537. <https://doi.org/10.1103/PhysRevA.56.4537>
- [13] Oza, Dipak H. "Phase shifts and resonances for electron scattering by He^+ below the $N=2$ threshold." PHYSICAL REVIEW A 33.2 (1986): 824. <https://doi.org/10.1103/PhysRevA.33.824>
- [14] Bachau, H. "Position and widths of autoionising states in the helium isoelectronic sequence above the $N=2$ continuum." Journal of Physics B: Atomic and Molecular Physics 17.9 (1984): 1771. <https://doi.org/10.1088/0022-3700/17/9/016>
- [15] Macias, A., and A. Riera. "Energies and widths of singlet and triplet S resonances of helium-like systems." Physics Letters A 119.1 (1986): 28-32. [https://doi.org/10.1016/0375-9601\(86\)90639-0](https://doi.org/10.1016/0375-9601(86)90639-0)
- [16] Chung, Kwong T., and C. D. Lin. "DOUBLY EXCITED STATES OF Li^+ BELOW THEN= 2 AND $N=3$ THRESHOLDS OF Li^{2+} ." Atomic data and nuclear data tables 69.1 (1998): 101-124. <https://doi.org/10.1006/adnd.1998.0772>

- [17] Ho, Y. K. "Autoionisation states of helium isoelectric sequence below the $n=3$ hydrogenic thresholds." *Journal of Physics B: Atomic and Molecular Physics* 12.3 (1979): 387. <https://doi.org/10.1088/0022-3700/12/3/016>
- [18] Ho, Yu-Kun et AK Bhatia. "Complex-coordinate calculation of 1,3 D resonances in two-electron systems." *PHYSICAL REVIEW A* 44.5 (1991) : 2895. <https://doi.org/10.1103/PhysRevA.44.2895>
- [19] Ivanov, I. A., and U. I. Safronova. "Calculation of the correlation part of the energy to two-electron systems." *Optics and spectroscopy* 75.3 (1993): 298-304.
- [20] Ivanov, P. B., and U. I. Safronova. "Correlation and relativistic effects for 3l3l' autoionization states." *Physica Scripta* 49.4 (1994): 408. <https://doi.org/10.1088/0031-8949/49/4/005>
- [21] Bhatia, A. K., and A. Temkin. "Calculation of autoionization of He and H⁻ using the projection-operator formalism." *Physical Review A* 11.6 (1975): 2018. <https://doi.org/10.1103/PhysRevA.11.2018>
- [22] Zhou, Zhongyuan, and Shih-I. Chu. "Spin-dependent localized Hartree-Fock density-functional calculation of singly, doubly, and triply excited and Rydberg states of He- and Li-like ions." *Physical Review A* 71.2 (2005): 022513. <https://doi.org/10.1103/PhysRevA.71.022513>
- [23] Ndao, A. S., et al. "High-lying resonance states of He and H." *The European Physical Journal D-Atomic, Molecular, Optical and Plasma Physics* 5.3 (1999): 327-334. <https://doi.org/10.1007/PL00021597>
- [24] Faye, N. A. B., et al. "Energy levels in the resonant photoionization of heliumlike Ne⁸⁺." *Physical Review A* 75.4 (2007): 042713. <https://doi.org/10.1103/PhysRevA.75.042713>
- [25] Ndao, A. S., et al. "Autodetaching singlet and triplet states of below the $N=4$ threshold of the residual hydrogen atom." *Journal of Physics B: Atomic, Molecular and Optical Physics* 31.16 (1998): 3489. <https://doi.org/10.1088/0953-4075/31/16/004>
- [26] Wagué, A. "Application of the diagonalization approximation to the $n=3$ resonant photoionization of helium-like systems." *Zeitschrift für Physik D Atoms, Molecules and Clusters* 6 (1987): 337-344. <https://doi.org/10.1007/BF01437060>
- [27] FANO, U. "Effects of Configuration Interaction on Intensities and Phase Shifts." *Phys. Rev.* 124 (1961): 1866-1878. <https://doi.org/10.1103/PhysRev.124.1866>
- [28] Kaminskii, A. A., et al. "Spectroscopic properties and stimulated emission in the $^4F_{3/2} \rightarrow ^4I_{11/2}$ and $^4F_{3/2} \rightarrow ^4I_{13/2}$ transitions of Nd³⁺ ions from cubic Bi₄Ge₃O₁₂ crystals." *physica status solidi (a)* 33.2 (1976): 737-753. <https://doi.org/10.1002/pssa.2210330234>
- [29] Senashenko, V. S., and A. Wague. "Resonance photoabsorption of the helium atom in the vicinity of the (3s3p)¹P resonance." *Journal of Physics B: Atomic and Molecular Physics* 12.8 (1979): L269. <https://doi.org/10.1088/0022-3700/12/8/002>
- [30] Wagué, A. "Calculation of the photo-electrons angular distribution asymmetry parameter β_{2p} near the (3s3p)¹P resonance of He." *Zeitschrift für Physik D Atoms, Molecules and Clusters* 8 (1988): 251-254. <https://doi.org/10.1007/BF01436948>
- [31] Butler, P. H., P. EH Minchin, and B. G. Wybourne. *Tables of hydrogenic Slater radial integrals*. Univ. of Canterbury, Christchurch, New Zealand, 1971. [https://doi.org/10.1016/S0092-640X\(71\)80004-9](https://doi.org/10.1016/S0092-640X(71)80004-9)