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The calculation of transition probabilities for atomic oxygen[⋆]

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Abstract. The atomic transition probabilities for multiplet and individual lines and oscillator strengths for multiplet lines between some triplet and quintet levels have been calculated using weakest bound electron potential model theory (WBEPMT) in neutral oxygen. The results obtained in this work are in good agreement with the data obtained from different theoretical methods given in the literature and with critically evaluated values taken from NIST. Moreover, some new transition probabilities and oscillator strengths for highly excited levels in atomic oxygen have been obtained using this method.

PACS. 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding – 32.70.Cs Oscillator strengths, lifetimes, transition moments

1 Introduction

The lighter elements with 4–10 electrons are astrophysically abundant and accurate atomic data such as absorption oscillator strengths, transition probabilities and lifetimes of excited levels are needed for the accurate interpretation of observational data. The atomic transition probabilities are perhaps the most important fundamental parameters in atomic spectroscopy. Their values affect the choice of transition utilized for analysis and the accuracy of many critical measurements such as temperature and atomic concentration [1–3]. Oxygen is an important element because of its presence in the Earth's atmosphere as well as in many astrophysical and laboratory spectra. For the analysis of the spectra and various other applications, radiative atomic quantities are required for all ionization stages [4]. Moreover, oscillator strengths for allowed transitions in atomic oxygen are required for the interpretation or modeling of many physical plasmas [5]. Thus, the optical properties of atomic oxygen are very important in both atmospheric and astrophysical applications.

Many methods have been proposed for experimental measurements or theoretical calculations of the transition probabilities and oscillator strengths in oxygen atom. Solarski and Wiese [6] have measured transition probabilities for six oxygen multiplets using wall-stabilized high-current arc technique and they obtained results agree with other theoretical and experimental methods. Samson and Petrosky [7] have measured continuum ionization transition probabilities using photoelectron spectroscopy technique for atomic oxygen. Jenkins [8] has measured the absorption oscillator strengths of (3P-3S) O I transitions at 130 nm using a line absorption method. Goldbach and Nollez [9] have measured oscillator strengths of 12 lines belonging to 5 multiplets in the 950–1200 Å spectral range of neutral oxygen with a wall-stabilized arc technique. Bridges and Wiese [10] have measured the transition probabilities for $3s\ {}^3\mathrm{S}^\circ - 4p\ {}^3\mathrm{P}$ and $3s\ {}^5\mathrm{S}^\circ - 4p\ {}^5\mathrm{P}$ multiplets in O I with wall-stabilized arc technique. Musielok et al. [11] have measured the transition probabilities of several multiplet pairs of C I, N I and O I. Pradhan and Saraph [12] have employed the bound-state wave functions obtained by the close-coupling method in frozen-cores approximation for oscillator strengths involving levels with quantum number $n \leqslant 4$ of neutral oxygen. Breit-Pauli results in MCHF approximation for transition data have been determined by Tachiev and Fischer for the nitrogen-like sequence (Z = 7–17) and oxygen-like sequence (Z = 8–20) [13]. Tayal and Henry [14] have calculated oscillator strengths using configuration interaction wave function for some allowed transitions of atomic oxygen. Bell and Hibbert [5] have calculated oscillator strengths using both the R-matrix and configuration interaction method for allowed transitions involving some symmetry for atomic oxygen. Hibbert et al. [15] have calculated atomic transition rates and f values in the triplet and quintet systems and for individual lines of neutral oxygen. They included about 450 configuration state functions for both upper and lower states in configuration interaction approach. Biemont et al. [16] have calculated oscillator strengths for $2p^3({}^4\mathrm{S}^\circ)nl - 2p^3({}^4\mathrm{S}^\circ)n'l'$ transitions taking configuration

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[⋆] Tables 1–3 are only available in electronic form at `http://www.epj.org`

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interaction and relativistic effect into account. They have used two different computer codes: the CIV3 configuration interaction code and the pseudo-relativistic Hartree-Fock program for calculating f-values. Using the atomic structure computer program SUPERSTRUCTURE, new accurate oscillator strengths have been calculated by Biemont and Zeippen [17] for $2p$–$3s$ and $3s$–$3p$ allowed transition in neutral oxygen. They have taken most important configuration interaction and relativistic effects into account. Opacity Project team [18] used an R-matrix code in conjunction with the close-coupling approximation for only multiplet states. Escalante and Victor [19] have presented f values and photo-ionization cross sections for dipole allowed transitions involving excited states of oxygen using open-shell model potential method that allows the calculation of excited-state single configuration wave functions. Nahar [4] has calculated photo-ionization cross sections, oscillator strengths and energy levels using the R-matrix method in close-coupling approximation of some oxygen ions. Jönsson and Godefroid [20] have calculated oscillator strengths for transitions between low-lying levels in atomic oxygen using Multi-Configurational Hartree-Fock (MCHF) method and configuration interaction (CI) method. Recently, Zheng et al. have used the WBEPM theory for calculation of physical parameters such as transition probabilities, oscillator strengths, lifetimes and energy levels of alkali metal atoms, heavy metal atoms and many valence electron atomic or ionic systems [21–30].

In this work, we have calculated transition probabilities and oscillator strengths for transitions between some triplet and quintet levels by using the WBEPM theory in atomic oxygen. Accuracy and reliability of the results which are calculated by using the WBEPM theory depend sensitively on the expectation values of radii. In order to calculate oscillator strengths and transition probabilities for transitions between further highly excited states than those obtained in previous works with well-known ab-initio methods, we used numerical non-relativistic Hartree-Fock method for expectation radii. The results presented in this theory are compared with data obtained from different theoretical methods and critical values in the NIST for determination of reliability of oscillator strength and transition probability results.

2 The method

The reliabilities of the values of transition probability and oscillator strength are mainly based on the performance of calculation methods used. The transition probabilities designate the statistical probability that an electron will spontaneously drop to a lower electronic state from an upper electronic state. The total electric dipole transition probability from to all levels of has been given [31]

$$A = \frac{64\pi^4 e^2 a_0^2 (E_{J'} - E_J)^3}{3h(2J'+1)} S \tag{1}$$

here, $(E_{J'} - E_J)$ is the energy difference between relevant levels and S is the electric dipole line strength. Moreover, energy and line strength apply for $(E_{J'} - E_J)$ in kaysers (cm^{-1}) and S in atomic units of $e^2 a_0^2$. Line strength is determined according to the coupling schemes and the transition types in atomic or ionic systems. The text book given by Cowan [31] has presented in details how the line strength can be calculated due to considered coupling schemes and for different type of transitions. The most important quantity for the calculation of S line strength is determination of the radial transition integral or transition matrix elements. In order to solve the radial parts of Schrödinger equation in multi electron systems, the several approximations must be imposed.

The WBEPM theory has been widely employed to calculate many of spectroscopic data in physical and chemical areas [23–26]. The weakest bound electron potential model theory has been developed by Zheng [21,22] and has been applied by Zheng et al. [23–30] for determination of some physical parameters in many-electrons atomic and ionic systems. He suggested a new model potential to describe the electronic motion in multi-electron systems and separated electrons within a given system into two groups, the weakest bound electron (WBE), and others (non-weakest bound electrons — NWBE). The WBE in many-electron systems is also the electron which can most easily be excited or ionized. Some atomic or ionic properties in multi-electron systems such as transition, excitation and ionization may be referred to weakest bound electron's behavior. The treatment of WBE gives accurate information about these properties. By the separation of the electrons in a given system, complex many-electron problem can be simplified as single electron problem and so can be solved easily [28–30].

According to the WBEPM theory, the radial wave function of the weakest bound electron can be obtained to be [28]

$$R_{nl}(r) = \left(\frac{2Z^*}{n^*}\right)^{l^*+3/2} \left[\frac{2n^*}{(n-l-1)!}\Gamma(n^*+l^*+1)\right]^{-1/2} \times \exp\left(-\frac{Z^* r}{n^*}\right) r^{l^*} L_{n-l-1}^{2l^*+1}\left(\frac{2Z^* r}{n^*}\right) \tag{2}$$

here, n^* and l^* parameters have been given to be

$$n^* = n + d, \quad l^* = l + d. \tag{3}$$

On the other hand, Z^*, n^*, l^* quantities are defined to be effective nuclear charge, effective principal quantum number, effective azimuthal quantum number, respectively, and d is an adjustable parameter. These parameters can be obtained by solving equations (4) and (5) together

$$I = -\varepsilon = \frac{Z^{*2}}{2n^{*2}} \tag{4}$$

$$\langle r \rangle = \frac{3n^{*2} - l^*(l^*+1)}{2Z^*} \tag{5}$$

here I is ionization energy and $\langle r \rangle$ is expectation value for radius of weakest bound electron. The ionization energies and expectation values for radii of all states must be known for the parameters Z^*, n^*, l^* to be determined. It is well-known that some difficulties in obtaining the parameters directly from theory are still present. Therefore, Zheng has suggested that the ionization energies for the weakest bound electron should be taken from experimental energy values in literature and expectation value of radius of the weakest bound electron is obtained from many different theoretical methods. After obtaining the relevant parameters, radial transition integral or radial matrix element between two different states can be determined easily using radial wave functions given in equation (2). For a transition from the level (n_i, l_i) to the level (n_f, l_f), the expectation value of r^k or radial transition integral for $k = 1$ can be obtained [28–30]

$$
\begin{aligned}
\langle n_i, l_i | \, r^k \, | n_f, l_f \rangle &= \int_0^\infty r^{k+2} R_{n_i l_i}(r) R_{n_f l_f}(r) dr \\
&= (-1)^{n_f+n_i+l_f+l_i} \left(\frac{2Z_f^*}{n_f^*} \right)^{l_f^*} \left(\frac{2Z_i^*}{n_i^*} \right)^{l_i^*} \\
&\times \left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*} \right)^{-l_f^*-l_i^*-k-3} \left[\frac{n_f^{*4} \Gamma(n_f^* + l_f^* + 1)}{4Z_f^{*3}(n_f - l_f - 1)} \right]^{-1/2} \\
&\times \left[\frac{n_i^{*4} \Gamma(n_i^* + l_i^* + 1)}{4Z_i^{*3}(n_i - l_i - 1)} \right]^{-1/2} \\
&\times \sum_{m_1=0}^{n_f-l_f-1} \sum_{m_2=0}^{n_i-l_i-1} \frac{(-1)^{m_2}}{m_1! m_2!} \left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*} \right)^{m_1+m_2} \\
&\times \left(\frac{Z_f^*}{n_f^*} + \frac{Z_i^*}{n_i^*} \right)^{-m_1-m_2} \Gamma(l_f^* + l_i^* + m_1 + m_2 + k + 3) \\
&\times \sum_{m_3=0}^{S} \binom{l_i^* - l_f^* + k + m_2 + 1}{n_f^* - l_f^* - 1 - m_1 - m_3} \\
&\times \binom{l_f^* - l_i^* + k + m_1 + 1}{n_i^* - l_i^* - 1 - m_2 - m_3} \\
&\times \binom{l_i^* + l_f^* + k + m_1 + m_2 + m_3 + 2}{m_3} \qquad (6)
\end{aligned}
$$

where, $S = \min\{n_f - l_f - 1 - m_1, n_i - l_i - 1 - m_2\}$ and $k > -l_f^* - l_i^* - 3$. The papers given by Zheng et al. described in detail WBEPM theory.

In this paper, we have used the weakest bound electron potential model theory in the calculation of radial transition matrix elements for determination of line strength. The parameters required in the evaluation of radial transition integral have been determined using two different wave functions.

3 Results and discussions

The atomic transition probabilities for multiplet-individual lines and oscillator strengths for multiplet lines between triplet and quintet levels of some transitions of neutral oxygen have been calculated using weakest bound electron potential model theory. In the determinations of parameters Z^*, n^*, l^*, we have employed both numerical non-relativistic Hartree-Fock (NRHF) wave functions [32] and numerical Coulomb approximation (NCA) wave functions [33] for expectation values of radii. Experimental ionization energies [34] have been used for needed energy level values. Then, transition probabilities and oscillator strengths have been calculated for many transitions in atomic oxygen. Our transition probability and oscillator strength results have been compared with results obtained from different theoretical methods and accepted values taken from NIST [35] which contain recommended values for many transitions. The NIST values are given together with their accuracy rating in relevant columns of tables. Experimental and theoretical data for comparisons are quite limited for especially highly excited transitions which are considered in this study. Therefore, some results obtained from our calculations have been compared only with NIST data.

Our results for multiplet oscillator strengths are given in Table 1 (see the *Supplementary Online Materials*). It can be seen from Table 1 that our results presented in this work for multiplet oscillator strengths calculated using WBEPM theory are in good agreement with different theoretical results given in the literature and accepted values from NIST. As results of these comparisons, it can be seen that the average agreement of our oscillator strength values is within 4.18% to the A-accuracy values taken from NIST. The transition probabilities between some triplet and quintet levels for atomic oxygen are given in Tables 2 and 3. Our results given in Tables 2 and 3 are compared with the accepted values from NIST [35] for many transitions, the ones obtained by Tachiev and Fischer [13] for some transitions belonging to lower levels from MCHF calculations and with Configuration Interaction calculations given in Hibbert et al. [15]. It can be seen from Tables 2 and 3 that our results are in good agreement with MCHF results, accepted values taken from NIST and Configuration Interaction results. The average agreement of our transition probability values for triplet levels is within 2.00% to the A-accuracy values taken from NIST, within 4.66% to the MCHF values and within 2.36% to the Configuration Interaction calculations. For quintet levels, average agreement is within 2.66% to the A-accuracy values taken from NIST, within 5.53% to the MCHF values and within 3.72% to the Configuration Interaction calculations. Moreover, some new transition probabilities and oscillator strengths for highly excited levels in atomic oxygen have been obtained using this method and are shown in the last few lines of tables.

The both theoretical and experimental determination of transition probabilities and oscillator strengths for multi-electron systems are an important but also difficult problem in atomic physics. While the calculation procedure for the systems with a few electrons can be carried out easily, the calculations become more difficult and complex in the case of increasing number of electrons. In atomic oxygen, there are six electrons apart from the $1s^2$

core electrons. Interactions among these valence electrons are complex and important. It is not easy to deal with these multi-electron systems since many configurations and orbital basis-set functions may be necessary to be taken into account to obtain accurate results. Therefore, many of the used methods have considered only low-lying levels which are very insufficient for practical and astrophysical applications. Moreover, some theoretical methods do not consider fine-structure effects and only provide multiplet results. It is seen from the literature that in the measurement of transition probabilities and oscillator strengths, there are still many experimental difficulties and certain measurements are generally restricted to transitions involving only low-lying levels. Thus, there is a need for further effort to obtain accurate data on transition probabilities, oscillator strengths and lifetimes of especially higher excited levels.

The weakest bound electron potential model theory is an efficient method especially for excited or highly excited transitions. The WBEPM theory uses the observed binding energy and expectation values of radii to find the effective values of nuclear charge, principal quantum number and orbital quantum number. Then, using Z^*, n^* and l^* parameters, radial wave functions can be produced easily. In this method, the calculation is carried out easily and in a shorter time for transitions belonging to both low lying and highly excited levels. The accuracy and reliability of the results calculated using the WBEPM theory strongly depends on the choice of wave functions used in determination of the expectation values of radii. Previously, we employed numerical NRHF wave functions for determination of relevant parameters in atomic lithium [36], nitrogen [37,38], fluorine [39] and obtained very satisfactory transition probability and oscillator strength results using WBEPM theory.

In the WBEPM theory, determinations of the parameters Z^*, n^* and l^* are sufficient for spectroscopic data calculations. These parameters are obtained using expectation values of radii and experimental energy values. Since experimental ionization energy data are very precise, determination of the expectation values of the radii is more crucial than energy values in the WBEPM theory. Thus, to obtain more sensitive and reliable results, we have employed the more sophisticated numerical non-relativistic Hartree-Fock (NRHF) wave functions rather than NCA wave functions which are commonly employed in the WBEPM theory literature. The deviation between real expectation values and values calculated from NCA method for the ground state and some excited states is very large. We have used NRHF wave functions in the determination of expectation values of the radius for the ground states. Moreover, the use of this theory leads to considerable savings in the computing time. Thus, this method allows the study of hundreds or thousands of transitions in a reasonably short time. Considering the agreement between our results and other results, unknown or new transition probabilities in both low lying and highly excited levels can be determined. The use of WBEPM theory is advantageous for much more complicated systems, especially for those in highly lying states. In this approximation, the values of the transition probabilities and oscillator strengths will be better if the expectation value of radius belonging to the levels is accurate enough.

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