Electron impact excitation of helium-like oxygen up to \( n = 4 \) levels including radiation damping

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Abstract
The primary x-ray diagnostic lines in He-like ions are mainly excited by electron impact from the ground level to the \( n = 2 \) levels, but at high temperatures \( n > 2 \) levels are also excited. In order to describe the atomic processes more completely, collision strengths are computed for O VII including for the first time all of the following: (i) relativistic fine structure, (ii) levels up to \( n = 4 \), and (iii) radiation damping of autoionizing resonances. The calculations are carried out using the Breit–Pauli \( R \)-matrix method with a 31-level eigenfunction expansion. Resonance structures in collision strengths are delineated in detail up to the \( n = 4 \) thresholds. For highly charged He-like ions radiation damping of autoionizing resonances is known to be significant in certain energy ranges. We investigate this effect in detail and find that while resonances are discernibly damped radiatively as the series limit \( n \to \infty \) is approached from below, the overall effect on effective cross sections and rate coefficients is found to be very small. Collision strengths for the principal lines important in x-ray plasma diagnostics, \( w, x, y \) and \( z \), corresponding to the four transitions to the ground level \( 1s^2(1S_0) \leftarrow 1s2p(1P^0_1), 1s2p(3P^0_2), 1s2p(3P^1_2), 1s2s(3S_1) \), are explicitly shown. Significant differences are found with previous works for several transitions. The contribution from the resonances converging to the levels from the complex \( n = 4 \) is found to be significant for some transitions and can increase the rate by a factor of four. This work is carried out as part of the Iron Project-RmaX Network.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
Helium-like ions provide the most important x-ray spectral diagnostics in high-temperature fusion and astrophysical plasmas. The new generation of x-ray satellites such as the Chandra X-Ray Observatory and the X-Ray Multi-Mirror Mission-Newton provide high-resolution spectra of different types of astronomical objects (e.g. Kaastra et al (2000), Porquet and Dubau (2000),
Porquet et al (2001)). The high sensitivity of these observatories and the high quality of the spectra they produce requires highly accurate atomic data for a precise interpretation. The aim of the Iron Project $R$-matrix calculations for x-ray spectroscopy (IP-RmaX) is to calculate extended sets of accurate collision strengths and rate coefficients for all ions of importance in x-ray diagnostics. Among previous works, the electron impact excitation of helium-like oxygen was previously considered by Pradhan et al (1981a, 1981b) in the distorted wave and close coupling (CC) approximations for transitions up to the $n = 2$ levels. Sampson et al (1983) and Zhang and Sampson (1987) used the Coulomb–Born approximation with exchange, intermediate coupling and some resonance effects to obtain collision strengths for helium-like ions, with atomic number $Z$ spanning a large range of values ($4 < Z < 74$). Kingston and Tayal (1983a, 1983b) calculated the collision strengths for two transitions, from the ground state to $2^3S_1$ and to $2^3P_0^e$, using the close coupling $R$-matrix (RM) method, and derived the corresponding effective collision strengths. Both the Pradhan et al and Kingston and Tayal calculations were in $LS$ coupling. The present work aims at generating a more complete dataset of high reliability for $Ovii$, including all important effects for highly charged ions such as relativistic effects, radiation damping and resonances in higher complexes up to $n = 4$.

The method and computations are summarized in section 2. Results for the collision strengths and important issues are discussed in section 3, and the present results for the effective (Maxwellian averaged) collision strengths are compared with previous calculations. The main conclusions are given in section 4, together with an estimate of the accuracy of the results.

2. Method and computations

The collisional calculation in this work has been carried out using the Breit–Pauli $R$-matrix (BPRM) method as used in the Iron Project (IP) and utilized in a number of previous publications. The aims and methods of the IP are presented in Hummer et al (1993). We briefly summarize the main features of the method and calculations.

In the coupled channel or CC approximation the wavefunction expansion, $\Psi(E)$, for a total spin and angular symmetry $SL\pi$ or $J\pi$, of the $(N+1)$ electron system is represented in terms of the target ion states as

$$\Psi(E) = A \sum_i \chi_i \theta_i + \sum_j c_j \Phi_j,$$

where $\chi_i$ is the target ion wavefunction in a specific state $S_1L_\pi \pi_i$ or level $J_i \pi_i$, and $\theta_i$ is the wavefunction for the $(N+1)$th electron in a channel labelled as $S_1L_\pi (J_\pi \pi)k^2_\ell (S_\pi \pi \pi)[J_\pi \pi]$; $k^2_\ell$ is the incident kinetic energy. In the second sum the $\Phi_j$ are correlation wavefunctions of the $(N+1)$ electron system that (a) compensate for the orthogonality conditions between the continuum and the bound orbitals, and (b) represent additional short-range correlations that are often of crucial importance in scattering and radiative CC calculations for each symmetry. The $\Phi_j$ are also referred to as ‘bound channels’, as opposed to the continuum or ‘free’ channels in the first sum over the target states. In the relativistic BPRM calculations the set of $SL\pi$ are recoupled in an intermediate (pair) coupling scheme to obtain $(e + \text{ion})$ states with total $J\pi$, followed by diagonalization of the $(N+1)$-electron Hamiltonian. Details of the diagonalization and the RM method are given in many previous works (e.g. Berrington et al 1995).

The target expansion for the CC calculations consists of 31 fine-structure levels arising from the 19 $LS$ terms with principal quantum number $n \leq 4$. The target eigenfunctions were developed using the SUPERSTRUCTURE program (Eissner et al 1974) in a version due to Nussbaumer and Storey (1978). The full expansion, together with the scaling factors in the Thomas–Fermi potential employed in SUPERSTRUCTURE, are given at the end of table 1.
Table 1. Energy levels compared with observed values from NIST (in Ryd). Spectroscopic configurations: 1s^2, 1s2s, 1s2p1s3s, 1s3p, 1s3d, 1s4s, 1s4p, 1s4d, 1s4f. Correlation configurations: 2s^2, 2p^2, 2s2p2s3s, 2s3p, 2s3d, 2s4s, 2s4p, 2s4d, 2s4f. Scaling factors: λ_1s = 0.9932, λ_2s = 1.0759, λ_2p = 0.9217, λ_3s = 1.0306, λ_3p = 0.9023, λ_3d = 0.9547, λ_4s = 1.0182, λ_4p = 0.9038, λ_4d = 0.9512, λ_4f = 1.0200.

| Conf | Levels   | $E_{\text{calc}}$ | $E_{\text{obs}}$ |
|------|----------|-------------------|------------------|
| 1s^2 | 1S_0     | 0.0000            | 0.0000           |
| 1s2s | 3S_1     | 41.2438           | 41.2315          |
| 1s2p | 3P_0     | 41.7933           | 41.7872          |
| 1s2p | 3P_1     | 41.7942           | 41.7877          |
| 1s2p | 3P_2     | 41.7997           | 41.7928          |
| 1s2s | 1S_0     | 48.6577           | 48.6509          |
| 1s3p | 3P_0     | 48.8114           | 48.8044          |
| 1s3p | 3P_1     | 48.8116           | 48.8044          |
| 1s3p | 3P_2     | 48.8132           | 48.8044          |
| 1s3s | 3S_0     | 48.8217           | 48.8112          |
| 1s3d | 3D_1     | 48.8930           | 48.8837          |
| 1s3d | 3D_2     | 48.8931           | 48.8842          |
| 1s3d | 3D_3     | 48.8935           | 48.8843          |
| 1s3d | 3D_4     | 48.8971           | 48.8937          |
| 1s3p | 3P_1     | 48.9281           | 48.9218          |
| 1s4s | 3S_0     | 51.1813           | 51.1798          |
| 1s4p | 3P_0     | 51.2436           | 51.2360          |
| 1s4p | 3P_1     | 51.2437           | 51.2360          |
| 1s4p | 3P_2     | 51.2444           | 51.2360          |
| 1s4s | 3S_0     | 51.2475           | 51.2410          |
| 1s4d | 3D_1     | 51.2767           | 51.2675          |
| 1s4d | 3D_2     | 51.2767           | 51.2600          |
| 1s4d | 3D_3     | 51.2769           | 51.2720          |
| 1s4f | 3F_2     | 51.2786           | 51.2698          |
| 1s4f | 3F_3     | 51.2785           | 51.2698          |
| 1s4f | 3F_4     | 51.2787           | 51.2698          |
| 1s4d | 3D_2     | 51.2790           | 51.2739          |
| 1s4f | 3F_2     | 51.2787           | 51.2755          |
| 1s4p | 3P_1     | 51.2916           | 51.2870          |

In order to estimate the quality of the target wavefunction expansion, we compare the energy levels with those from the National Institute for Standards and Technology (NIST 2002) in table 1. A better criterion for the accuracy of the wavefunctions is the accuracy of the oscillator strengths for transitions in the target ion. In table 2 we compare the $gf$-values with the evaluated compilation from NIST for a number of dipole transitions in O VII. For the energies the agreement with the NIST values is found to be very good, within 0.05% for all levels. The oscillator strengths agree well within 10% (however, for some of the values given by NIST, the estimated accuracy is 30%). Another accuracy criterion is the level of agreement between the oscillator strengths in the length and the velocity formulations, which we also find to be a few per cent for all transitions. The Einstein $A$-values are also presented in table 2 to enable ready application of the present collisional data in radiative-collisional models for spectral diagnostics (e.g. Porquet and Dubau (2000), Porquet et al (2001)).

The 19 LS terms are recoupled in the relativistic BPRM calculations into the corresponding 31 fine-structure levels up to the $n = 4$ complex using the routine RECUPD that performs...
 intermediate coupling operations including the one-body Breit–Pauli operators (Hummer et al 1993). The reconstructed target eigenfunctions and the resulting target energies reproduce to \(10^{-5}\) Ryd the results from SUPERSTRUCTURE, verifying that the algebraic operations have been carried out self-consistently and without loss of accuracy. The collision strengths have been calculated for electron energies \(0 \leq E \leq 200\) Ryd. This wide energy range ensures a good coverage of the region where resonances up to the \(n = 4\) complex are important, as well as the higher energy region where no resonances have been included (all channels are open) but where the background collision strengths still make a significant contribution to the Maxwellian averaged rate coefficient for electron temperatures of interest.

The inner region RM basis set included 50 orbitals per angular momentum. Because of the importance of the near-threshold resonances in the Maxwellian average rate coefficient, careful attention has been devoted to the resolution and a precise mesh has been chosen. A mesh of \(10^{-4}\) Ryd was selected for the region where resonances are important, and a coarser mesh for the region where all channels are open. We included the contribution to the collision strengths from all symmetries with total angular momentum \(J\) and both odd and even parities, \(J \pi \leq (\frac{3}{2})^{1/2}\). The contribution of higher partial waves was included using the Coulomb–Bethe approximation via the ‘top-up’ facility in the asymptotic region program STGF of the RM package (Burke and Seaton (1986); modified by Eissner and Chen).

| Term, Term | \(E_1\) (Ryd) | \(E_2\) (Ryd) | \(A_{H}^{NIST}\) (s) | \(A_{cal}^{NIST}\) (s) | \(g \times f_{H}^{NIST}\) | \(g \times f_{cal}^{NIST}\) |
|-----------|-------------|-------------|----------------|----------------|----------------|----------------|
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
| 1s2–1s2p  | 1s2–1s3p   | 1s2–1s3p   |
3. Results and discussion

In figures 1 and 2 we present the collision strengths for transitions from the ground state to levels in the \( n = 2 \) complex, and to levels in the complex \( n = 3 \) respectively. The high resolution of the calculations with a large number of points allows us to resolve clearly all the resonances up to the last threshold in the \( n = 4 \) complex. We delineate the Rydberg series converging to the different series limits in all three complexes. In both figures 1 and 2, the identification of the Rydberg series converging to \( n = 3 \) and \( n = 4 \) thresholds has been marked. The doubly excited \( \text{(e + O vii)} \rightarrow \text{O vi resonance complexes, KMM, KMN etc, converging towards the different n = 3 and 4 levels are clearly resolved. We can anticipate from figure 2 that, for some transitions, the low magnitude of the background and the high density of the resonances will make the contribution of these resonances converging to the n = 4 complex very important and dominant. This is confirmed by our work (discussed later).} \)
Figure 2. Collision strengths for transitions from the ground state to levels within the complex with principal quantum number $n = 3$. $1s^2 \, ^1S_0 \rightarrow 3^1S_1$, $3^3P_1$, $3^3P_2$, $3^3D_1$, $3^3D_2$, $3^3D_3$, $3^1P_1$.

3.1. Radiation damping

It has previously been shown (Presnyakov and Urnov 1979, Pradhan 1981, Pradhan and Seaton 1985) that radiation damping may have a significant effect on the resonances in collision strengths for highly charged ions since the radiative decay rates may be large and may compete with autoionization rates, i.e. the effect of dielectronic recombination on electron impact excitation. We studied in detail the radiation damping effect of dielectronic recombination on resonance structures, collision strengths and rate coefficients. In figures 3 and 4, we present the Rydberg series converging to the $n = 2$ and 3 levels coupled to the ground state $1^1S_0$ via strong dipole transitions, $2 \, ^1P_1$ (figure 3) and $3 \, ^1P_1$ (figure 4). Since the autoionization rates decrease as $n^{-3}$, and the radiative rate remains constant, radiation damping increases with $n$ and the resonances are wiped out as the series limit is reached. We illustrate the effect for one total $(e + \text{ion})$ symmetry $J\pi = 1^\circ$. It can be seen how effective the diminishing of resonances is as we approach the threshold. The overall effect of damping on the averaged collision strength can be up to a factor of two (figure 5). However, the region where the effect is important is very small, just below the threshold of convergence. It is called the ‘quantum
Electron impact excitation of helium-like oxygen up to \( n = 4 \) levels including radiation damping

Figure 3. Partial collision strengths for transitions from ground state 1s\(^2\) 1S\(_0\) to 2\(^1\)P\(_2\), 2\(^3\)S\(_0\), 2\(^1\)S\(_0\). Dashed curve: resonance for \( J\pi = 1_{\text{even}} \) converging to 2\(^1\)P\(_2\); solid curve: resonance for \( J\pi = 1_{\text{even}} \) converging to 2\(^1\)P\(_0\) damped by recombination.

defect region’, since we use the Bell and Seaton (1985) (see also Pradhan and Seaton (1985)) multi-channel quantum defect theory in this region. In figures 4 and 5 this region corresponds to \( \Delta E = 0.36 \text{ Ryd} \) (\( \nu_{\text{min}} = 10 \)). Overall, however, we find that for O\( VIII \) the effective collision strengths and the rate coefficients are not significantly affected (figures 6 and 7). Indeed, in figure 6, damped and undamped effective collision strength \( \Upsilon \) curves are indistinguishable (solid curve).

Figures 4 and 5 show that below threshold the collision strength is constant. This is due to the high value of the effective quantum number reached in our calculations (\( \nu \approx 100 \)), sufficient to illustrate graphically the effect of radiation damping up to the region where the resonances are almost completely damped. In order to resolve all resonances converging to the different thresholds of interest, we used a \( \nu \)-mesh with about 1000 points for each interval (\( \nu, \nu + 1 \)). In the quantum defect region the Coulomb potential dominates the scattering
In order to directly demonstrate the effect of radiation damping in figures 4 and 5, we show that the collision strengths converge toward the background value calculated neglecting the long-range non-dipole potentials. However, just above the threshold the potential is not only Coulombic but multipole contributions are also important. In order to isolate the effect we switched off the multipole contributions so that there is continuity across the threshold and only the radiation damping effect is illustrated.

3.2. Effective collision strengths

The Maxwellian averaged collision strengths

\[ \Upsilon(T) = \int_{0}^{\infty} \Omega_{ij}(\epsilon_j) e^{-\epsilon_j/kT} d(\epsilon_j/kT), \]
Electron impact excitation of helium-like oxygen up to $n = 4$ levels including radiation damping

![Graphs](image)

**Figure 5.** Total averaged collision strengths for transitions from ground state $1s^2 1S_0$ to $2^3S_1$, $2^3P_0, 2^3P_2, 2^1S_0$ between $2^3S_0$ and $2^3P_0$ thresholds. Dashed line: no damping; solid curve: damping effect.

have been computed for all transitions among levels up to $n = 4$. As has been shown for He-like Fe xxv (Kimura et al 1999, 2000, Machado-Pelaez et al 2002) the resonances arising from the complex $n = N + 1$ have a strong effect on transitions to the complex $n = N$. Along with the full calculation including all the 31 fine-structure states up to $n = 4$, we considered a smaller target model, including all 17 levels up to $n = 3$ to compare the effect of the resonances. Figures 6–8 show the effective collision strengths for transitions from the ground state to the $n = 2$ levels, as well as transitions among levels of the $n = 2$ complex, and transitions from the ground level and levels of the $n = 2$ complex to levels of the $n = 3$ complex. We find that for some transitions the contribution from the higher $n = 4$ resonances gives rise to a factor of two increase in the effective collision strengths at the temperature of maximum abundance of O vii ($T \approx 2 \times 10^6$ K) and even larger at lower temperatures. As shown previously it affects transitions to and within the $n = 3$ complex. But we found that some transitions within the
Figure 6. Effective collision strengths for the principal lines (z, x, y, w). solid curve: this work (long dashed curve on (b) x and y; solid = $1S \leftarrow 2P^0$) dot–dashed curve: Kingston and Tayal (1983b) short-dashed curve: Zhang and Sampson (1987), crosses: Pradhan et al (1981a). Note: the two curves with and without radiation damping effect are indistinguishable (solid curve).

$n = 2$ complex are also significantly affected. In figure 8, transitions from $n = 1$ to 3, from $n = 2$ to 3 and within $n = 2$ and 3 complexes are all significantly enhanced by the resonances converging to $n = 4$ levels, and in a large range of temperatures.

We compared the effective collision strengths with previous calculations for the principal curves w, x, y, z (figures 6(a), (b) and (d)), corresponding to the four transitions to the ground level $1s^2(1S_0) \leftarrow 1s2p(^3P^0_1), 1s2p(^3P^0_2), 1s2p(^3P^0_1), 1s2s(^3S_1)$ respectively, that are of primary interest in x-ray spectral diagnostics (e.g. Gabriel and Jordan (1969), Pradhan (1982), Porquet et al (2001)). Some other transitions are also compared where the data are available in literature. Illustrative results are presented for the four principal curves (figure 6) as well as four other transitions within the $n = 2$ complex (figure 7).

Generally, the agreement between the different calculations, depending on the transition and temperature, is between 10 and 30%. However, for some transitions the differences are larger in some temperature ranges. Basically, these differences stem from
Electron impact excitation of helium-like oxygen up to $n = 4$ levels including radiation damping

Figure 7. Effective collision strengths for transitions within the $n = 2$ complex. Solid curve: this work, dashed curve: Zhang and Sampson (1987), crosses: Pradhan et al (1981a); (c) shows the total collision strength including the fine-structure transitions $2^3S_1 - 2^3P_{0,1,2}$. (i) the coupling effects due to the $n = 3$ and 4 levels in the CC expansion, (ii) relativistic effects included through the Breit–Pauli approximation, (iii) improved delineation of resonances with high-resolution, and (iv) ensuring convergence with complete ‘top-up’ of partial waves.

All of these four factors are important in determining the final effective collision strength.

In figure 6 we present the transition from the ground level to the different fine structure levels with $n = 2$. The z-line (figure 6(a)) presents some significant difference with previous calculations, especially at low temperatures. There is about 35% difference with Pradhan et al (1981a, crosses) and between 15 and 30% with Kingston and Tayal (1983b, dot–dashes) for $T < 2 \times 10^5$ K. Above $7 \times 10^5$ K the difference is within 10% with Kingston and Tayal (1983b, dot–dashes) but the present work is systematically 15–20% below Pradhan’s values. The agreement with Zhang and Sampson (1987, short dashed curve) is very good for the high temperature if, as recommended in their article, one adds the contribution from resonances of
the $n = 2$ complex as, for example, from Steenman-Clark and Faucher (1984). The primary cause of differences with previous works is the resolution of complexes of resonances near threshold, \textit{in between the $n = 2$ levels}, where high resolution is crucial and detailed fine structure plays an important role. The $\Omega_{1ij}$ at low energies determines the effective collision strength at low temperatures since $\Upsilon_{ij}(T \to 0) = \Omega_{1ij}(E \to 0)$. The importance of the resonances for this transition was already shown by Pradhan et al (1981b) and Kingston and Tayal (1983a, 1983b) in their $LS$ coupling calculations. The present results demonstrate the need for a relativistic and high-resolution calculation in order to obtain accurate excitation rates at low temperatures.

With the exception of Zhang and Sampson (1987), the previous works did not consider fine structure. Therefore, the effective collision strengths for the $1^1S_0 - 2^3P_0^0$ transitions, corresponding to the forbidden and intercombination curves $x$ and $y$, are shown individually in figure 6(b), as well as added together with the contribution from the third level $2^3P_0^0$. The
difference with all others is no more than 20% at all temperatures.

For the dipole-allowed transition (1 1S0–21Po), corresponding to the w-line, the high-temperature rates are within 10%. But still, the low-temperature rates are higher by 25% than those from Pradhan et al (1981a).

The strong dipole transitions among the excited n = 2 levels (23S1–23Po and 21S0–21Po) (figures 7(c) and (d)) are very important in spectral diagnostics calculations since they enable the collisional coupling at high electron densities that affects the x, y, and z curves. This also has implications for the competition between the effect of collisional redistribution among these lines, and photoexcitation by background ultraviolet radiation, if present in the x-ray source (e.g. Porquet et al (2001)). The total multiplet collision strength for this transition is in good agreement with earlier works except for the transition 23S1–23S0. For temperatures in the range [2 × 10^5–2 × 10^6], corresponding to the temperatures of maximum abundance for O vii in photoionized or coronal plasmas, the effective collision strengths of Pradhan et al are overestimated by 30% compared to the present work, which agrees well with Zhang and Sampson (1987).

4. Conclusions

The general conclusions of the paper are as follows.

(1) The most complete CC calculation to date using the BPRM method has been carried out for helium-like oxygen, including resonances up to n = 4 levels. Detailed studies of radiation damping indicate that it may have a significant effect on the detailed collision strengths in a small energy region below the threshold(s) of convergence, but not on the effective collision strengths. Radiation damping is marginally important for higher-Z elements since the transition probabilities increase with Z; Pradhan (1983a, 1983b) has found the effect on the z-transition to be about 9% in ϒ for Fe xxv close to the temperature of maximum abundance of helium-like iron.

(2) It is verified that the effects of coupling and resonances from the n = N + 1 complex play an important role in effective collision strengths for the transitions to the complex n = N. It is also found that it significantly affects transitions to other complexes (n = N – 1 in this case) and not only the n = N complex.

(3) The new results for the important x-ray line transition may significantly affect the analysis of O vii x-ray spectra from photoionized sources (e.g. active galactic nuclei), where O vii may be abundant at relatively low temperatures. In collisional ionized (coronal) sources the new results may not affect the theoretically computed line intensities significantly at temperatures close to maximum abundance, but should still do so at lower temperatures. It would be preferable to employ the present data in future collisional-radiative and photoionization models.

(4) As all relevant atomic effects in electron–ion collisions have been considered, and resonances have been carefully delineated, we should expect our results to be of definitive accuracy. Nonetheless, we conservatively estimate the precision to be about 10–20%.

(5) All data will be electronically available from the first author from delahaye@astronomy.ohio-state.edu.

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