Effects of LS term dependence in He-like ions

D. C. Griffin
Department of Physics, Rollins College, Winter Park, Florida 32789

D. M. Mitnik and M. S. Pindzola
Department of Physics, Auburn University, Auburn, Alabama 36849

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In this paper, we report on the effects of LS term dependence on radiative rates and electron-impact excitation cross sections in He-like ions. In particular, we examine the variation of the $2p$ orbital between the $1s2p\ ^3P$ and $1s2p\ ^1P$ terms in Li^+, C^{4+}, F^{7+}, and Mg^{10+}. We find that for transitions between the $1s2p\ ^1P_1$ level and the ground state, term dependence causes a variation in both the radiative rate and the excitation cross section at nearly the twenty percent level; however, by Mg^{10+} this variation is less than five percent.

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In almost all close-coupling calculations of electron-impact excitation, a unique set of orthonormal $n\ell$ orbitals must be used to represent all the atomic states of the target. However, there are a number of situations where, within a given configuration, there is significant variation in certain radial orbitals from one LS term to another. For example, this term dependence is often quite pronounced in sp, p^5d, and d^9f configurations [1,2]. A classic case is the $2s2p$ configuration in neutral Be, where the average radius of the $2p$ orbital associated with the ^3P term is 2.9 a.u., while the average radius of the $2p$ orbital for the ^1P term is 5.0 a.u. [1]. These effects are due to unusually large exchange interactions—thus they become much less pronounced in $nsn'p$, $np^5n'd$, and $nd^9n'f$ configurations, if n' is much larger than n, or in $nsnp$, np^5nd, and nd^9nf configurations in intermediate and high-charge-state ions.

In this paper we will focus on the $1s2p$ configuration in He-like ions. We initiated this study after performing an extensive set of R-matrix close-coupling calculations of excitation cross sections and configuration-interaction calculations of radiative rates in Mg^{10+} [3]. In this ion, we found that term-dependent effects were negligible but wondered about how important they might be in lower charge-state He-like ions. In general, one would not expect term dependence to be very important in $1s2p$ configurations because of the large separation between the $1s$ and $2p$ orbitals and the corresponding reduction in the exchange interaction [1]. Even though the variation of the $2p$ orbital between the ^3P and ^1P terms in He-like ions is indeed small compared to the example of the $2p$ orbital in neutral Be given above, as we shall see, it is large enough to have a pronounced effect on the electron-impact excitation and the radiative transition between the $1s2p\ ^1P_1$ level and the ground state for the lower charged species.

This is important for two primary reasons. In close-coupling calculations of electron-impact excitation in these ions, $1sn\ell$ configurations with n up to 4 are typically included in the description of the target [4]. Some of the term-dependence in the $2p$ orbital will then be included through configuration interaction of $1s2p\ ^1P$ with both $1s3p\ ^1P$ and $1s4p\ ^1P$. However, as we shall see, this provides only a partial correction. Second, both electron-impact excitation and ionization in He-like ions are now being studied using advanced close-coupling techniques such as the R matrix with pseudostate (RMPS) method. For example, Brown *et al.* [6] completed an RMPS calculation on Li^+ in which they included in their close-coupling expansion spectroscopic states through $n=3$ plus 34 pseudostates to represent the high Rydberg states and the continuum. They attributed the difference between their results and the earlier 19-state results of Berrington and Nakazaki [4] for excitation to the $1s2p\ ^1P$ term to coupling to the continuum. However, we would now argue that a large part of this difference is due to the additional term dependence included in the RMPS calculations through configuration interaction between $1s2p\ ^1P$ and the ^1P pseudostates [5]. As we shall show, it is not due to coupling to the continuum since it can be incorporated through the addition of a single pseudostate, which is not included in the close-coupling expansion but only in the configuration-interaction expansion of the target.

We have made three calculations of electron-impact excitation cross sections and radiative rates for each ion. However, because of the limited number of states included in these calculations they should be considered only model calculations designed specifically to investigate the importance of term dependence in these ions. All radial wave functions were determined using Frose Fischer's Hartree-Fock programs [7] and all scattering calculations were performed using a modified version of the RMATRIX I atomic scattering package [8].

In all electron-impact excitation calculations, we included only the $1s^2\ ^1S$, $1s2s\ ^3S$, $1s2s\ ^1S$, $1s2p\ ^3P$, and $1s2p\ ^1P$ terms in the close-coupling (CC) expansion. These calculations differed only in the orbitals and the configuration-interaction (CI) expansions used to describe the target. In order to remove any resonances attached to terms included in the CI expansion, but not the CC expansion, we used the pseudostate elimination method of Gorczyca *et al.* [9]. Finally we determined cross sections between individual levels using the intermediate-coupling frame transformation (ICFT) method [10]. It is based on the use of quantum-defect theory to generate unphysical K matrices in LS coupling. These unphysical K matrices are then transformed to intermediate

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TABLE I. Electric dipole radiative rates (A_r) for the $1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0$ and the $1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$ transitions for Li^+, C^{4+}, F^{7+}, and Mg^{10+}, calculated using: the CA basis set, the CACI basis set, and the TD basis set in comparison to the results of relativistic many-body theory (RMBT) calculations.

Transition	CA A_r (Hz)	CACI A_r (Hz)	TD A_r (Hz)	RMBT[a] A_r (Hz)
Li^+				
$(1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0)$	1.61×10^4	1.63×10^4	1.66×10^4	1.79×10^4
$(1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0)$	3.02×10^{10}	2.80×10^{10}	2.52×10^{10}	2.56×10^{10}
C^{4+}				
$(1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0)$	2.66×10^7	2.68×10^7	2.70×10^7	2.83×10^7
$(1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0)$	9.72×10^{11}	9.38×10^{11}	8.93×10^{11}	8.86×10^{11}
F^{7+}				
$(1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0)$	1.74×10^9	1.75×10^9	1.77×10^9	1.83×10^9
$(1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0)$	5.93×10^{12}	5.80×10^{12}	5.63×10^{12}	5.57×10^{12}
Mg^{10+}				
$(1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0)$	3.21×10^{10}	3.23×10^{10}	3.26×10^{10}	3.38×10^{10}
$(1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0)$	2.04×10^{13}	2.01×10^{13}	1.97×10^{13}	1.95×10^{13}

[a]Johnson *et al.* [12].

coupling using term-coupling coefficients; finally, the physical K matrices are determined from the unphysical K matrices and level energies using standard quantum-defect theory. In all calculations, $J\Pi$ partial waves from $J=0.5$ to $J=18.5$ were included and then topped up as follows: the dipole transitions were topped-up using a method originally described by Burgess [11] for LS coupling and implemented here in intermediate coupling; the nondipole transitions were topped-up assuming a geometric series in J.

For our first basis set, we generated the $1s$ and $2p$ orbitals from a configuration-average Hartree-Fock (CAHF) calculation on the $1s2p$ configuration and the $2s$ orbital from a CAHF calculation on $1s2s$ configuration. We then corrected the $1s$ orbital in the $1s^2$ ground configuration by performing a multiconfiguration Hartree-Fock (MCHF) calculation in which we minimized the energy of the $1s^2\ ^1S$ term by varying the $\overline{3s}$ pseudo-orbital in a MCHF expansion that included the $1s^2\ ^1S$, $1s2s\ ^1S$, and $1s\overline{3s}\ ^1S$ terms. We refer to this as our configuration-average (CA) basis; it does not include any term dependence in the $2p$ orbital. The radiative rates for the CA basis were then determined from a Breit-Pauli CI calculation that included the five even levels arising from the $1s^2$, $1s2s$, and $1s\overline{3s}$ configurations and the four odd levels arising from the $1s2p$ configuration.

Our second basis set was the same as that described above, except that we added the levels associated with the $1s3p$ and $1s4p$ configurations, for which the $3p$ and $4p$ orbitals were also determined from CAHF calculations. Through configuration interaction between the terms of the $1s2p$ configuration and the terms of the $1s3p$ and $1s4p$ configurations, this basis set includes a partial correction for term dependence in the $2p$ orbital, as would be the case in a much larger close-coupling calculation that included the $1s3\ell$ and $1s4\ell$ configurations in both the CC and CI expansions. We refer to this as our configuration-average with configuration-interaction (CACI) target basis. The radiative rates for the CACI basis were determined from a Breit-Pauli CI calculation that included the five even levels of the CA basis and the 12 odd levels arising from the $1s2p$, $1s3p$, and $1s4p$ configurations.

The third basis set included an exact treatment of term dependence in the $2p$ orbital. The $1s$ and $2p$ orbitals were first determined from a Hartree-Fock calculation on the $1s2p\ ^3P$ term and the $2s$ orbital was generated from a CAHF calculation on the $1s2s$ configuration. We corrected the $1s$ orbital in the $1s^2$ ground state using a $\overline{3s}$ pseudo-orbital as described above. Finally we corrected the $2p$ orbital for term-dependence by generating a $\overline{3p}$ pseudo-orbital from an MCHF calculation that included the $1s2p\ ^1P$ and $1s\overline{3p}\ ^1P$ terms and in which the energy of the $1s2p\ ^1P$ term was minimized by varying only the $\overline{3p}$ orbital. We refer to this as a term-dependent (TD) target basis. The radiative rates for this basis were determined from a Breit-Pauli CI calculation that included the five even levels arising from the $1s^2$, $1s2s$, and $1s\overline{3s}$ configurations and the eight odd levels arising from the $1s2p$ and the $1s\overline{3p}$ configurations.

The radiative rates for the $1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0$ and $1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$ transitions, calculated in the length gauge using the three basis sets described above are presented in Table I. As can be seen, the variation between the results of our three calculations is small for the $1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0$ transition for all stages of ionization. However, term dependence causes a much larger variation between the radiative rates for the $1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$ transition. The difference between the rates determined using the CA and TD basis in Li^+ is nearly 17%; however, as one would expect, it decreases with ionization stage and is less than 4% in Mg^{10+}. Furthermore, we see by comparing the results of the CACI calculations with the other two that less than 50% of the correction of the CA basis for term dependence is provided by the configuration interaction of $1s2p\ ^1P$ with $1s3p\ ^1P$ and $1s4p\ ^1P$. In this table, we also show the radiative rates for these ions as determined from the much more sophisti-

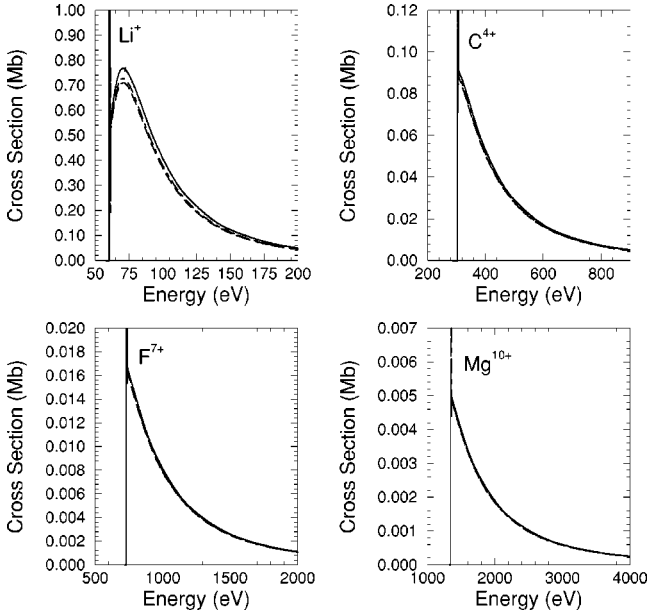

FIG. 1. Electron-impact excitation cross sections for the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^3P_1$ transition in Li^+, C^{4+}, F^{7+}, and Mg^{10+}. Dashed lines, calculated using the CA basis; dot-dashed lines, calculated using the CACI basis; solid lines calculated using the TD basis.

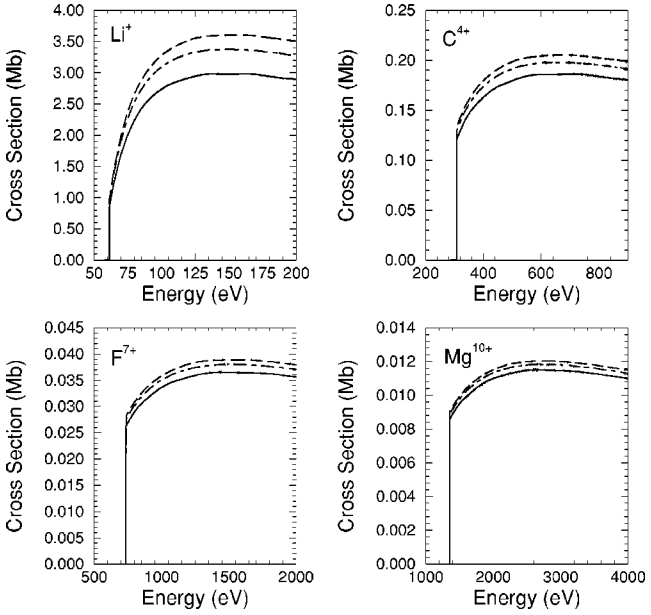

FIG. 2. Electron-impact excitation cross sections for the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^1P_1$ transition in Li^+, C^{4+}, F^{7+}, and Mg^{10+}. Dashed lines, calculated using the CA basis; dot-dashed lines, calculated using the CACI basis; solid lines calculated using the TD basis.

cated relativistic many-body theory (RMBT) calculations of Johnson *et al.* [12]. In light of the simplicity of the TD basis, it is surprising that the radiative rates from our term-dependent calculation are as close as they are to the RMBT results.

Similar results are found in the electron-impact excitation cross sections shown in Fig. 1 for the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^3P_1$ excitation and in Fig. 2 for the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^1P_1$ transition. The spikes in the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^3P_1$ cross sections at threshold are due to resonances attached to the $1s2p\ {}^1P_1$ level. With the exception of Li^+, the three calculated cross sections for the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^3P_1$ transition are difficult to distinguish on the scale of the graphs; for Li^+, the TD result differs from the CA result by about 8% at the peak in the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^3P_1$ nonresonant cross section, while for Mg^{10+} they differ by less than 2% at energy just below the narrow resonance at threshold. However, the differences between the calculated cross sections for the $1s^2\ {}^1S_0 \rightarrow 1s2p\ {}^1P_1$ excitation are much more substantial. The difference between the CA and TD cross section for Li^+ is about 18% and it gradually decreases as a function of ionization stage to about 4% for Mg^{10+}. We also notice that the CACI calculations account for less than 50% of the reduction in the cross section due to term dependence.

These results indicate that any close-coupling calculations of electron-impact excitation in the lower charge states of He-like ions, that do not include a large number of pseudostates in the CC expansion, should explicitly include in the CI expansion those pseudostates that are needed to correct for term dependence in the $1snp\ {}^1P$ levels. These effects will be most important for excitation to $1s2p\ {}^1P_1$, but will persist to a smaller degree in the excited $1snp\ {}^1P_1$ levels. Furthermore, in order to properly assess the effects of coupling to the continuum on excitation cross sections to the $1snp\ {}^1P_1$ levels, RMPS calculations for low charge state He-like ions should be compared to smaller close-coupling calculations that include in the CI expansion those pseudostates needed to correct for term dependence in the ${}^1P_1$ levels.

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[1] C. Froese Fischer, *The Hartree-Fock Method for Atoms* (Wiley, New York, 1977), pp. 91–94.

[2] D.C. Griffin and M.S. Pindzola, Comments At. Mol. Phys. **13**, 1 (1983).

[3] D. M. Mitnik, M. S. Pindzola, and D. C. Griffin, Phys. Rev. A **62**, 062711 (2000).

[4] K.A. Berrington and S. Nakazaki, J. Phys. B **24**, 1411 (1991).

[5] One might expect the effects of coupling to the continuum to have a quite different energy dependence than the effects of term dependence. However, in most cases this is not true. Coupling to the continuum often begins far below the ionization limit, close to the excitation threshold, making this effect on the excitation cross quite similar in appearance to that of term dependence. For example, see D.C. Griffin, N.R. Badnell, and M.S. Pindzola, J. Phys. B **33**, 1013 (2000).

[6] G.J.N. Brown, M.P. Scott, and K.A. Berrington, J. Phys. B **32**, 737 (1999).

[7] C. Froese-Fischer, Comput. Phys. Commun. **64**, 369 (1991).

[8] K.A. Berrington, W.B. Eissner, and P.H. Norrington, Comput. Phys. Commun. **92**, 290 (1995).
[9] T.W. Gorczyca, F. Robicheaux, M.S. Pindzola, D.C. Griffin, and N.R. Badnell, Phys. Rev. A **52**, 3877 (1995).
[10] D.C. Griffin, N.R. Badnell, and M.S. Pindzola, J. Phys. B **31**, 3713 (1998).
[11] A. Burgess, J. Phys. B **7**, L364 (1974).
[12] W.R. Johnson, D.R. Plante, and J. Sapirstein, Adv. At. Mol. Phys. **35**, 255 (1995).