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The study of the core–valence and core–core correlation effects on the radiative properties along the magnesium isoelectronic sequence

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ABSTRACT

We investigated the effect of core–valence and core–core correlations on the energy levels and transition probabilities along the Mg isoelectronic sequence from Si^{2+} to U^{80+}. In order to attain a certain accuracy for the atomic structure we considered configurations obtained by electron promotions from the $n = 3$ up to $n = 7$ valence shells. Core–valence and core–core correlations are systematically included in the model by allowing single and double electron promotions from the $n = 2$ core up to the $n = 6$ and $n = 5$ shells with $l \leq 4$ and $l \leq 2$, respectively. The present results contain the energy of the levels arising from the valence configurations along with oscillator strengths and radiative rates corresponding to $E1$, $M1$, $E2$, $M2$ transitions between states arising from $3l3l'$ with $l, l' \leq 2$ and $3snl''$ with $n \leq 7$ and $l'' \leq 4$ configurations. We conclude the data accuracy trend along the magnesium isoelectronic sequence as a result of the detailed study of the correlation effects on the radiative properties. The core–valence correlations generally improve both energy and radiative rate values, while the core–core correlations mostly give better oscillator strengths but may slightly increase the energy deviations. The calculations have been performed by employing the fully relativistic model-potential Flexible Atomic Code.

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Contents

1. Introduction

Transitions belonging to the Mg-like ions are useful for performing diagnostics of astrophysical [1–3] and laboratory plasmas [4–8]. The necessity for accurate data led to a series of calculations for excitation energy, line strengths and transition probabilities by employing the multiconfiguration Hartree–Fock (MCHF) [9,10], Dirac–Fock (MCDF) [11], Dirac–Hartree–Fock (MCDHF) [12], random-phase approximation [13] and configuration-interaction (CI) using Breit–Pauli (BP) [14–16] methods. The sequence itself is interesting from a theoretical standpoint since there are two electrons outside the complete neon core meaning that core–valence and core–core correlations play an important role in the atomic calculations [17] along with the many-body effects [18]. The $3s^2(^1S_0)$, $3p^2(^1S_0)$, $3d^2(^1S_0)$ configuration interaction (CI) is dominant in the calculation and strong mixing also occurs between the $3p^2(^1D_2)$ and $3s3d(^1D_2)$ terms, while the transition probabilities are significantly affected by the degree of electron correlation [19]. Resonant lines such as $3s^2(^1S_0)$–$3s3p(^1P_1^o)$ play a crucial role in electron-impact excitation processes [20] and accurate calculation requires inclusion of more than valence–valence correlations [21].

In recent years the Mg-like ions have been subjected to different calculations using various methods. The *R*-matrix intermediate-coupling frame transformation (ICFT) approach [22] has been employed by L. Fernandez Menchero et al. [23] to compute the structure and electron-impact collision strengths for the magnesium like ions from Al II to Zn XIX. Only valence–valence correlations have been accounted for by using 283 levels arising from $3snl$, $3pnl$ and $3dnl$ configurations with $n \leq 5$ and $l \leq 4$. Reasonable agreement with experimental results has been reached.

The MCDHF approach [24] has been used by F. Hu et al. [25] to compute energy levels and radiative transition probabilities for the Mg-like ions ranging from $Z = 19$ to 92. The $1s^22s^22p^6$ neon core was kept fixed while the active set was systematically increased by including configurations belonging to the $n = 3$ complex up to $n = 7$, each time optimizing the orbitals. In order to account for core–valence correlations, the same procedure was applied using core-excited reference sets obtained by exciting an electron up to $n \leq 4$ from either $2p$ or $2s$ orbital. Good agreement between the computed atomic data for the $n = 3$ to $n' = 3$ transitions and results from NIST [26] has been attained.

The MCDHF approach has been also employed recently by S. Gustafsson et al. [27] to accurately compute energy levels, lifetimes and transition rates belonging to the Ca IX to As XXII and Kr XXV Mg-like ions. The states arise from the multireference set containing the following configurations: $3l3l'$ with $l, l' \leq 2$, $3l4l'$ with $l \leq 2, l' \leq 3$ and $3s5l$ with $l \leq 4$. Single and double excitations to orbital sets with principal quantum number $n = 6, 7, 8$ have been allowed while keeping the $1s$ shell closed. Only single excitations have been allowed from the $2p$ and $2s$ inner subshells.

A finite configuration interaction (CI) expansion can be chosen to well account for the near-degeneracy effect or static correlation, but in order to include the bulk of dynamic correlations one needs to consider a significantly large-scale CI expansion [28]. An alternative approach to adopting large-scale configuration interaction (CI) expansions is that of relativistic many-body perturbation theory (MBPT). The multi-reference Møller–Plesset (MR-MP) many-body perturbation theory [18] was used by J.A. Santana [29] to compute with unprecedented accuracy low-lying energy levels within the magnesium isoelectronic sequence from $Z = 12$ to $Z = 100$. The multi-reference configuration interaction (MR-CI) calculations have been performed for the $3s^{n1}3p^{n2}3d^{n3}$ configurations with $\sum_{i=1}^{3} n_i = 3$ accounting for the near-degeneracy effect while state-specific MR-MP calculations based on this CI expansion were performed in order to treat the residual electron correlation. Quantum electrodynamical effects were included by estimating the electron self-energy and the vacuum polarization.

The relativistic MBPT has been employed by U.I. Safronova et al. [30] to obtain excitation energies, radiative rates and lifetimes within the Mg-like ions for Z ranging from 13 to 100. The Breit interaction has been considered within the effective Hamiltonian and the electric dipole allowed transitions corresponding to the $n = 3$ complex have been calculated in both length and velocity gauges.

Despite the necessity for knowledge of emission lines in plasma diagnostics, only few papers treat the forbidden transitions within the Mg-like ions. Y. Zou and C. Froese Fischer [12] used different optimization strategies for the intercombination $3s^2(^1S_0)$–$3s3p(^3P_1^o)$ transition belonging to Mg-like Al II to S V ions. As a result, they managed to eliminate the transition probabilities dependence on optimization strategies and they further extended their calculations to magnetic dipole ($M1$), electric ($E2$) and magnetic ($M2$) quadrupole transitions between the $3s^2(^1S_0)$, $3s3p(^3P_{0,1,2}^o)$, $3s3p(^1P_1^o)$ levels belonging to Mg-like ions with $Z \leq 92$ [31]. A comprehensive work on Na-like to Ar-like isoelectronic sequences performed by C. Froese Fischer et al. [19] also provides rates for selected $M1$, $E2$, $M2$ transitions belonging to Mg-like Mg I to Fe XV ions. More radiative rates for forbidden transitions are available from G. Tachiev and C. Froese Fischer [32].

There are no measured values available for $M1$, $E2$ and $M2$ transitions belonging to Mg-like ions to the authors knowledge. Forbidden $M1$ transition probabilities have been computed by A.M. Naqvi [33] by combining the Slater theory with the observed energy data. By comparing the empirically determined Slater parameters with the theoretically derived ones, he choose the values that resulted in better agreement between theory and experiment and then used them to compute the rest of the term intervals [34].

In a previous work, we computed the atomic structure and electron-impact collision strengths for the Mg-like S V ion while considering the effect of core–valence correlations by including 22 configuration-state function obtained by electron promotion from 2p subshell [35]. This improved the overall accuracy of the energy levels and transition probabilities as compared to other works from

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