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Contribution of near threshold states to dielectronic recombination in recombining plasma with Li-like Al ions

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ABSTRACT

The dielectronic recombination of Li-like into Be-like aluminum ions, in laser-produced plasmas with Li-like ions, is re-visited with respect to the contribution of near-threshold states. Results are shown for recombining laser-produced plasma regime. The relativistic Dirac *R*-matrix calculation is performed to output resonance energy levels and rates. The target energies, and orbitals, are calculated with the extended average level multi-configurational Dirac–Fock method in the general-purpose relativistic atomic structure package (GRASP), while for determining the plasma population densities distribution over the excited Rydberg states, the Atomic Data Analysis System (ADAS) package programs is used.

1. Introduction

The possible role of the negative-energy resonances on cross sections and rates for dielectronic recombination (DR) process in Mg^{8+} and C^{3+} into the plasma, has been recently pointed out [1,2]. The idea is that, depending on plasma density and temperature, there are different paths for an atomic ion to *temporarily* capture an electron into a high Rydberg state. In a realistic picture, i.e. in a plasma environment, due to collision processes, the electron energy is not constant varying with a thermal distribution. Then, different doubly excited states mix through configuration interaction (CI). Since, up to now, these below-threshold resonances have not been included in dielectronic recombination calculations, the experimental verification of their role is important.

In the present work we study another species that could be experimentally investigated from the point of view of the role of negative-resonances states to DR cross section and rate. We refer to laser-produced plasma with Li-like Al ions. This plasma has been studied in context of X-ray laser experiments, based on the recombination pumping scheme. Amplification of X–UV radiation has been experimentally demonstrated many years ago [3]. The amplified output signal has been detected along the axis of an elongated-shape plasma whose length (typically a few centimeters) is much larger than its transverse size (a few tenths of millimeter). The gain values have been inferred from the rate of exponential-growth of the amplified line-intensity with plasma length. In parallel with the experiments, computer modeling has also been performed. It has been demonstrated [4] the role of DR process on gain of X-ray lasers with Li-like ions when the electron temperature is of order of the $1s^22s - 1s^22p$ transition energy. The complete simulation of the gain coefficient (time- and space-dependent density and temperature being taken into account), for the radiation of spectral lines corresponding to 3d-5f ($\lambda = 10.57$ nm), 3d-4f ($\lambda = 15.46$ nm), and 4f-5g ($\lambda = 33.47$ nm) transitions, have then been examined with, and without, dielectronic recombination.

The electron scattering with Li-like Al has been subject of our previous works [5,6]. In the present work, the Dirac-Atomic – *R*-matrix relativistic calculation of atomic data for Al X is reported. We used the extended average level (EAL) multi-configurational Dirac–Fock (MCDF) method including quantum electrodynamics effects (QED) in the general-purpose relativistic atomic structure package (GRASP), while for determining the radiative and autoionizing rates the Dirac-Atomic *R*-matrix Code (DARC) was used. We restrict ourselves to including the only ten non relativistic configuration state functions: $1s^22s^2$, $1s^22p^2$, $1s^22s8s$, $1s^22s8d$, $1s^22s8f$, $1s^22s8g$, $1s^22p8s$, $1s^22p8p$, $1s^22p8f$, and $1s^22p8g$ in the calculation. This gives rise to 74 fine structure levels. To stabilize the order of the levels (odd or even), an initial analysis on each parity has been done. For the even parity group, the reference set contains {$1s^22s^2$, $1s^22p^2$, $1s^22s8s$, $1s^22s8d$, $1s^22s8g$, $1s^22p8p$ and $1s^22p8f$}, and for the odd parity groups {$1s^22s8p$, $1s^22p8s$, and $1s^22p8d$}. Once the order has been stabilized, we refer to $\Delta n = 0$, $n = 8$ transitions. There are not level energy data in the NIST table [7]. To check the accuracy of the resonance positions we used the Opacity Table [8]. The paper is structured as follows: In Section 2 we briefly outline the theoretical background of the calculations and present

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some details of the models for target states. In the Dirac-Atomic *R*-matrix scheme the internal region is treated similarly to a simple Dirac–Fock atomic structure calculation. The relativistic approach based on the Dirac equation has the advantage that all the relativistic effects are included not only for the eigen energies but, most importantly, in the radial wave functions. In the present calculation we included Breit interaction in the bound–bound part of the continuum Hamiltonian. The effect is to modify the thresholds and move the resonance structures. In Section 3 we give our results on DR rate for selected transitions allowing explicitly for resonance effects. Section 4 is devoted to conclusions.

2. Theory and details of calculations

The theoretical basis for the present calculations has been described in detail elsewhere [9-11]. It is essentially the relativistic or Dirac version of the *R*-matrix method. The *R*-matrix theory commences by partitioning configuration space into three regions describing the scattering of an electron by an *N*-electron atom or ion: an internal region, an external region and an asymptotic region. The *R*-matrix radius is chosen so that electron exchange between the colliding electron and the target vanishes and hence the colliding electron moves only in the long-range local multipole potential of the target. The solutions obtained in each of these regions are related by the *R*-matrix which corresponds to the inverse of the logarithmic derivative of the wave function on the boundary of the two regions. One important point to note is that, in the *R*-matrix method, the inner region solution is obtained only once, and then cross sections for any number of energy points are readily available. In the asymptotic region, the radius is propagated to a new distance, chosen large enough that the radial functions which represent the colliding electron can be accurately represented by an asymptotic expansion. The *K*-matrix elements and the *S*-matrix elements, and therefore the collision strengths Ω_{ij} can be easily calculated by matching the solution of the inner and outer regions at the *R*-matrix boundary radius $r = a$.

The Dirac Hamiltonian for the (*N*+1)-electron system, in atomic units, is written as:

$$H^{N+1} = \sum_{i=1}^{N+1} -ic\alpha\cdot\nabla_i + (\beta-1)c^2 - \frac{Z}{r_i} + \sum_{j=i+1}^{N+1}\frac{1}{|\mathbf{r}_j-\mathbf{r}_i|} \tag{1}$$

where i and j index the individual electrons, Z is the charge of an infinitely heavy point nucleus, the electron mass has been subtracted, and α and β are the usual Dirac matrices constructed from Pauli spin and unit matrices. The first three one-electron terms in the Hamiltonian are a momentum term, mass term and the electron-nucleus Coulomb attraction. The final two-electron term is the Coulomb electron–electron repulsion.

The Oxford code, the GRASP multiconfiguration Dirac–Fock (MCDF) code [12] was used to obtain the wave functions and energies of the Li-like Al target. We are interested in evaluating atomic data as level energies, radiative transition probabilities, line strengths and the Auger rates, for transitions between the $n = 8$ levels. To this end, configurations such that $1s^22s^2$, $1s^22p^2$, $1s^22s8s$, $1s^22s8d$, $1s^22s8f$, $1s^22s8g$, $1s^22p8s$, $1s^22p8p$, $1s^22p8f$, and $1s^22p8g$ have been included in the average level (EAL) calculation, while $1s^2$, $2s^2$ and $2p^2$ shells were kept full. These *jj*-coupled configuration state functions (CSF's) result in a set of 74 levels that are limited to the following symmetry–parity combinations $J^\Pi = 0^\pm$, $1^\pm$, $2^\pm$,$3^\pm$, $4^\pm$, 5^+.

In the isolated-resonance and independent process approximation, the dielectronic recombination cross section, as function of the free electron energy ε, for a given *N* electron initial level i through an intermediate (*N*+1) electron intermediate level j is given by [2]:

$$\sigma_j(\varepsilon) = \frac{\pi^2}{|E_{ji}|}\frac{g_j}{2g_i}\frac{\frac{\Gamma_j}{2\pi}}{(\varepsilon-E_{ji})^2+\frac{\Gamma_j^2}{4}}\sum_k \Gamma_A(j\to k)B_j \tag{2}$$

where E_j is the energy and g_j is the statistical weight of the (*N*+1) electron doubly excited level, E_i is the energy and g_i is the statistical weight of the *N* electron initial target level, and $E_{ij} = E_j - E_i$. The branching ratio for radiative stabilization is given by:

$$B_j = \frac{\sum_n \Gamma_R(j\to n)}{\sum_k \Gamma_A(j\to k)+\sum_n \Gamma_R(j\to n)} \tag{3}$$

where the radiative Γ_R and autoionizing Γ_A rates are evaluated using relativistic calculations. When a single state is embedded in a continuum or Rydberg series, the short range *S*-matrix has the property [13]:

$$1-|S_{11}(E)|^2 = \frac{\Gamma_R\Gamma_A}{(E-E_r)^2+[(\Gamma_R+\Gamma_A)/2]^2} \tag{4}$$

where E_r is the energy of the compact state (which can be positive or negative). Γ_A is related to the configuration interaction coupling between the state and the channel. This form does not depend on whether E_r is positive or negative. If the resonance is at positive energy, the rate coefficient for DR from a thermal distribution is calculated as:

$$K_d = \left(\frac{2\pi}{T}\right)^{3/2}\frac{2J_r+1}{2(2J_c+1)}\frac{\Gamma_R\Gamma_A}{\Gamma_R+\Gamma_A}e^{-E_r/T} \tag{5}$$

where T is the temperature ($T >> \Gamma_R + \Gamma_A$), J_r is the angular momentum of the resonance, and J_c is the angular momentum of the core. If the resonance is at negative energy, the probability to be in an n manifold with total angular momentum J_r and core electrons with angular momentum J_c is [1]:

$$P(n,J_r) = \left(\frac{2\pi}{T}\right)^{3/2}\frac{2J_r+1}{2(2J_c+1)}\exp(-E_n/T)\zeta(E_n) \tag{6}$$

where $E_n = -Z^2/(2(n^2)$ is the energy of the n manifold and $\zeta(E_n)$ is the Saha–Boltzmann deviation factor [14] depending on plasma temperature and density.

Table 1
Al^{9+} even-parity resonance-level energies. a^{-b} reads $a \times 10^b$.

Configuration	Term	Energy (au)	$\Gamma_R(s^{-1})$	$\Gamma_A(s^{-1})$
$1s^22p8p$	$^1P_1$	−0.02047	3.8703^{08}	2.822^{09}
	$^1S_0$	−0.01422	6.9516^{08}	5.295^{09}
	$^3P_2$	−0.01722	4.2001^{08}	1.245^{10}
	$^3P_1$	−0.01767	7.0116^{08}	7.405^{09}
	$^3P_0$	0.01871	9.2774^{08}	1.400^{09}
	$^3D_3$	0.00853	8.6016^{08}	7.777^{09}
	$^3D_2$	0.01387	4.5127^{08}	3.306^{09}
	$^3D_1$	0.00812	7.0136^{08}	3.351^{09}
	$^1D_2$	0.01071	6.9823^{08}	5.690^{09}
	$^3S_1$	0.01098	4.4253^{08}	6.782^{09}
$1s^22p8f$	$^1D_2$	−0.00566	4.0077^{08}	8.213^{08}
	$^1F_3$	−0.006465	3.6733^{08}	1.396^{08}
	$^3F_4$	−0.00573	3.6598^{08}	3.1799^{08}
	$^3F_3$	−0.00599	6.2259^{08}	6.807^{08}
	$^3F_2$	0.02429	5.2742^{08}	1.144^{09}
	$^3G_5$	0.02236	7.8005^{08}	5.174^{12}
	$^3G_4$	0.02149	4.0514^{08}	2.624^{06}
	$^3G_3$	0.02222	4.7989^{08}	7.795^{08}
	$^1G_4$	0.02358	1.6928^{08}	3.1741^{07}
	$^3D_1$	0.02365	9.8594^{08}	2.462^{08}
	$^3D_2$	0.02519	6.7174^{08}	1.6845^{08}
	$^3D_3$	0.02117	3.2497^{08}	2.055^{08}