Autoionizing Rates for Excited States of Many-Electron Ions

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1 Introduction

The most important difference between autoionization states and other excited states is an additional broadening of levels caused by the decay of these states (e.g. $2\ell n\ell' \Rightarrow 1skl''$). One can express the autoionizing widths of a level as the square of the decay amplitude:

$$, ^N(aLS, a'LS) = \sum_{a_0kl} \gamma(aLS, a_0klLS)\, \gamma(a'LS, a_0klLS), \tag{1}$$

where

$$\gamma(aLS, a_0klLS) = \sqrt{\frac{2\pi}{k}} \left\langle aLS \left| \sum_{i>j} 1/r_{ij} \right| a_0klLS \right\rangle . \tag{2}$$

Here k is the momentum of the ejected electron in the continuum state (a_0klLS), and aLS describes the autoionizing state. When a nonrelativistic basis is used, relativistic corrections must be taken into account perturbatively. A nonrelativistic basis was used for calculations of autoionization rates in the MZ code [1]–[2], in the model-potential method (SUPERSTRUCTURE code) [3], and in the multiconfiguration Hartree-Fock method (Cowan code [4]).

The purpose of this paper is to obtain simple formulas for autoionization rates for any atomic system by averaging over (LSJ). These calculations will be carried out using screened hydrogenic wave functions. The purpose of these calculations is to provide accurate, but easily used, atomic data.

2 Results and Discussion

Autoionization changes the state of two atomic electrons which initially can belong to either two different groups or to the same group of equivalent electrons. One of the electrons makes a transition to the continuous spectrum, and the other changes its state in the atom. Therefore, to calculate the probability of an autoionizing decay in a general multi-electron ion, it is sufficient to study the change of state in two systems: $(n_1l_1)^{p_1}(n_2l_2)^{p_2}(n_3l_3)^{p_3}$ and $(n_1l_1)^{p_1}(n_2l_2)^{p_2}$. We must study two types of transitions:

$$\begin{aligned} (n_1l_1)^{p_1}(n_2l_2)^{p_2}(n_3l_3)^{p_3} \Rightarrow &\quad (n_1l_1)^{p_1-1}(n_2l_2)^{p_2-1}(n_3l_3)^{p_3+1}k\ell \\ (n_1l_1)^{p_1}(n_2l_2)^{p_2} \Rightarrow &\quad (n_1l_1)^{p_1-2}(n_2l_2)^{p_2+1}k\ell \,. \end{aligned} \tag{3}$$

For LS averaged autoionization decay probabilities, one obtains in each case:

$$\begin{aligned} , ^N\left[(n_1l_1)^{p_1}(n_2l_2)^{p_2}(n_3l_3)^{p_3} \Rightarrow (n_1l_1)^{p_1-1}(n_2l_2)^{p_2-1}(n_3l_3)^{p_3+1}k\ell\right] = \\ p_1p_2\left(1 - \frac{p_3}{N_3}\right) A(n_1l_1n_2l_2; n_3l_3k\ell)\,, \end{aligned} \tag{4}$$

and

$$, ^N\left[(n_1l_1)^{p_1}(n_2l_2)^{p_2} \Rightarrow (n_1l_1)^{p_1-2}(n_2l_2)^{p_2+1}k\ell\right] = \frac{1}{2}p_1(p_1-1)\left(1-\frac{p_2}{N_2}\right)A(n_1l_1n_1l_1;n_2l_2k\ell)\,, \tag{5}$$

where $N_i = 2(2l_i+1)$ and where $A(n_1l_1n_2l_2;n_3l_3k\ell)$ is the two-electron decay probability.

$$\begin{aligned} & A(n_1l_1n_2l_2;n_3l_3kl_4) \\ = \; & \frac{2\pi}{k}(2l_3+1)(2l_4+1)\sum_l\left[\frac{1}{(2l+1)}P_l^2(n_1l_1n_2l_2;n_3l_3kl_4)+\frac{1}{(2l+1)}P_l^2(n_1l_1n_2l_2;kl_4n_3l_3)\right. \\ & \left. -\sum_{l'}\left\{\begin{array}{ccc} l_1 & l_4 & l' \\ l_2 & l_3 & l \end{array}\right\}P_l(n_1l_1n_2l_2;n_3l_3kl_4)P_{l'}(n_1l_1n_2l_2;kl_4n_3l_3)\right] \end{aligned} \tag{6}$$

$$\begin{aligned} A(n_1l_1n_1l_1;n_3l_3kl_4) \; = \; & \frac{2\pi}{k}\frac{(4l_1+1)}{(2l_1+1)}(2l_3+1)(2l_4+1)\sum_l\left[\frac{2}{(2l+1)}P_l^2(n_1l_1n_2l_2;n_3l_3kl_4)\right. \\ & \left. -\sum_{l'}\left\{\begin{array}{ccc} l_1 & l_4 & l' \\ l_1 & l_3 & l \end{array}\right\}P_l(n_1l_1n_1l_1;n_3l_3kl_4)P_{l'}(n_1l_1n_1l_1;kl_4n_3l_3)\right] \end{aligned} \tag{7}$$

Here P_l can be described as a product of a radial integral and 3j-Wigner coefficients:

$$P_l(n_1l_1n_1l_1;n_3l_3kl_4) = R_l(n_1l_1n_1l_1;n_3l_3kl_4)(-1)^{l+(l_1+l_2+l_3+l_4)/2}\left(\begin{array}{ccc} l_1 & l_4 & l \\ 0 & 0 & 0 \end{array}\right)\left(\begin{array}{ccc} l_2 & l_3 & l \\ 0 & 0 & 0 \end{array}\right) \tag{8}$$

Results of our calculations of $A(n_1l_1n_2l_2;n_3l_3kl_4)$ and $A(n_1l_1n_1l_2;n_3l_3kl_4)$ are given in Tables 1 and 2 for n_1l_1, n_2l_2 with $7 \geq n_1 \geq 1$, $(n_1-1) \geq l_1 \geq 0$, $7 \geq n_2 \geq 1$, $(n_2-1) \geq l_2 \geq 0$. The value of n_3 was chosen such that $\sqrt{\frac{1}{n_3^2}-\frac{1}{n_1^2}-\frac{1}{n_2^2}} > 0$ and $(n_3-1) \geq l_3 \geq 0$. The value of l_4 was defined by the triangle rule for the 3j-Wigner coefficient in Eq. (9). The value of k was given by $k = \frac{Z}{Z-\sigma}\sqrt{\frac{1}{n_3^2}-\frac{1}{n_1^2}-\frac{1}{n_2^2}}$, where Z is the nuclear charge and σ is a screening constant.

In total, 8116 kinds of $A(n_1l_1n_2l_2;n_3l_3kl_4)$ and $A(n_1l_1n_1l_2;n_3l_3kl_4)$ were calculated. We have selected the results with the largest values of A for illustration.

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References

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Table 1: Autoionizing rates $A(n_1l_1n_2l_2; n_3l_3kl_4)$ in s^{-1} as function of Z and σ

$n_1l_1n_2l_2$	$n_3l_3kl_4$	$Z=26$ $\sigma=0$	$Z=26$ $\sigma=1$	$Z=16$ $\sigma=1$	$Z=10$ $\sigma=1$	$Z=6$ $\sigma=1$	$Z=6$ $\sigma=2$
$2s2s$	$1sks$	2.057E+14	2.004E+14	1.968E+14	1.908E+14	1.785E+14	1.364E+14
$2s2p$	$1skp$	6.088E+13	5.886E+13	5.753E+13	5.533E+13	5.098E+13	3.691E+13
$2p2p$	$1sks$	1.039E+13	9.544E+12	9.014E+12	8.184E+12	6.716E+12	3.316E+12
$2p2p$	$1skd$	1.245E+14	1.160E+14	1.104E+14	1.016E+14	8.548E+13	4.511E+13
$2s3s$	$1sks$	2.604E+13	2.528E+13	2.477E+13	2.390E+13	2.212E+13	1.613E+13
$2s3p$	$1skp$	1.736E+13	1.667E+13	1.621E+13	1.545E+13	1.396E+13	9.349E+12
$2p3s$	$1skp$	1.252E+13	1.220E+13	1.199E+13	1.162E+13	1.084E+13	7.853E+12
$2p3p$	$1skd$	2.381E+13	2.208E+13	2.097E+13	1.918E+13	1.591E+13	7.845E+12
$2s4s$	$1sks$	1.050E+13	1.018E+13	9.964E+12	9.599E+12	8.852E+12	6.346E+12
$3s3s$	$1sks$	1.284E+13	1.245E+13	1.218E+13	1.172E+13	1.078E+13	7.601E+12
$3p3p$	$2pkp$	2.805E+14	2.776E+14	2.757E+14	2.723E+14	2.654E+14	2.394E+14
$3p3d$	$2pkd$	1.576E+14	1.565E+14	1.558E+14	1.545E+14	1.517E+14	1.402E+14
$3d3d$	$2pkf$	4.147E+14	4.057E+14	3.997E+14	3.895E+14	3.688E+14	2.981E+14
$3s3s$	$2pkp$	3.169E+13	3.106E+13	3.063E+13	2.988E+13	2.828E+13	2.212E+13
$3s3p$	$2pks$	8.273E+13	8.207E+13	8.162E+13	8.084E+13	7.922E+13	7.306E+13
$3s3d$	$2pkf$	1.811E+13	1.823E+13	1.831E+13	1.846E+13	1.878E+13	2.019E+13
$3p3d$	$2pks$	1.839E+13	1.791E+13	1.758E+13	1.704E+13	1.595E+13	1.239E+13
$3p3d$	$2pkg$	1.138E+13	1.130E+13	1.125E+13	1.115E+13	1.090E+13	9.623E+12
$3d3d$	$2pkp$	3.333E+13	3.251E+13	3.196E+13	3.104E+13	2.918E+13	2.303E+13
$3s4p$	$2pks$	1.794E+13	1.768E+13	1.750E+13	1.719E+13	1.655E+13	1.411E+13
$3p4s$	$2pks$	3.325E+13	3.261E+13	3.216E+13	3.141E+13	2.985E+13	2.418E+13
$3p4p$	$2pkp$	7.195E+13	7.028E+13	6.915E+13	6.723E+13	6.328E+13	4.941E+13
$3p4d$	$2pkd$	5.530E+13	5.411E+13	5.330E+13	5.190E+13	4.896E+13	3.810E+13
$3d4p$	$2pkd$	4.024E+13	4.021E+13	4.015E+13	3.994E+13	3.919E+13	3.367E+13
$3d4d$	$2pkp$	1.042E+13	9.845E+12	9.470E+12	8.863E+12	7.716E+12	4.557E+12
$3d4d$	$2pkf$	9.831E+13	9.423E+13	9.150E+13	8.692E+13	7.781E+13	4.963E+13
$3d4f$	$2pkg$	4.169E+13	3.854E+13	3.653E+13	3.336E+13	2.765E+13	1.390E+13
$3p5s$	$2pks$	1.665E+13	1.625E+13	1.598E+13	1.552E+13	1.456E+13	1.114E+13
$3p5p$	$2pkp$	3.318E+13	3.225E+13	3.161E+13	3.054E+13	2.835E+13	2.081E+13
$3p5d$	$2pkd$	2.643E+13	2.570E+13	2.520E+13	2.434E+13	2.256E+13	1.627E+13
$3d5p$	$2pkd$	1.731E+13	1.742E+13	1.746E+13	1.746E+13	1.719E+13	1.422E+13
$3d5d$	$2pkf$	4.263E+13	4.067E+13	3.934E+13	3.711E+13	3.264E+13	1.909E+13
$3d5f$	$2pkg$	2.425E+13	2.221E+13	2.091E+13	1.887E+13	1.524E+13	6.866E+12
$3p6p$	$2pkp$	1.828E+13	1.772E+13	1.734E+13	1.669E+13	1.538E+13	1.092E+13
$3p6d$	$2pkd$	1.479E+13	1.433E+13	1.402E+13	1.349E+13	1.239E+13	8.578E+12
$3d6d$	$2pkf$	2.276E+13	2.168E+13	2.094E+13	1.969E+13	1.718E+13	9.609E+12
$3d6f$	$2pkg$	1.450E+13	1.323E+13	1.242E+13	1.115E+13	8.892E+12	3.793E+12
$3p7p$	$2pkp$	1.120E+13	1.084E+13	1.059E+13	1.018E+13	9.340E+12	6.502E+12
$3d7d$	$2pkf$	1.369E+13	1.303E+13	1.258E+13	1.181E+13	1.025E+13	5.587E+12
$4p4p$	$2pkp$	2.440E+13	2.366E+13	2.316E+13	2.231E+13	2.057E+13	1.454E+13
$4p4d$	$2pkd$	1.351E+13	1.332E+13	1.316E+13	1.288E+13	1.218E+13	8.990E+12
$4d4d$	$2pkf$	2.875E+13	2.722E+13	2.619E+13	2.449E+13	2.116E+13	1.153E+13
$4d5d$	$2pkf$	1.117E+13	1.054E+13	1.012E+13	9.419E+12	8.040E+12	4.119E+12

Table 2: Autoionizing rates $A(n_1l_1n_2l_2; n_3l_3kl_4)$ in s^{-1} as function of Z and σ

$n_1l_1n_2l_2$	$n_3l_3kl_4$	$Z=26$ $\sigma=0$	$Z=26$ $\sigma=1$	$Z=16$ $\sigma=1$	$Z=10$ $\sigma=1$	$Z=6$ $\sigma=1$	$Z=6$ $\sigma=2$
$4f5f$	$3dkg$	1.647E+14	1.626E+14	1.612E+14	1.587E+14	1.534E+14	1.338E+14
$4s5d$	$3dks$	1.572E+13	1.565E+13	1.560E+13	1.551E+13	1.533E+13	1.464E+13
$4p5d$	$3dkp$	2.090E+13	2.081E+13	2.075E+13	2.064E+13	2.040E+13	1.947E+13
$4d5s$	$3dks$	3.719E+13	3.697E+13	3.682E+13	3.656E+13	3.600E+13	3.385E+13
$4d5p$	$3dkp$	4.649E+13	4.619E+13	4.599E+13	4.564E+13	4.491E+13	4.205E+13
$4d5d$	$3dkd$	8.276E+13	8.211E+13	8.166E+13	8.090E+13	7.928E+13	7.309E+13
$4d5f$	$3dkf$	8.039E+13	7.983E+13	7.944E+13	7.878E+13	7.735E+13	7.172E+13
$4d5g$	$3dkg$	1.309E+13	1.291E+13	1.279E+13	1.259E+13	1.217E+13	1.076E+13
$4f5p$	$3dks$	1.263E+13	1.232E+13	1.212E+13	1.178E+13	1.108E+13	8.755E+12
$4f5p$	$3dkd$	7.060E+12	7.362E+12	7.569E+12	7.922E+12	8.659E+12	1.133E+13
$4f5d$	$3dkp$	1.789E+13	1.752E+13	1.728E+13	1.686E+13	1.602E+13	1.312E+13
$4f5d$	$3dkf$	6.984E+13	6.990E+13	6.992E+13	6.993E+13	6.987E+13	6.858E+13
$4f5f$	$3dkd$	1.575E+13	1.548E+13	1.529E+13	1.497E+13	1.432E+13	1.203E+13
$4f5g$	$3dkh$	9.714E+13	9.476E+13	9.317E+13	9.049E+13	8.509E+13	6.713E+13
$4d6s$	$3dks$	2.084E+13	2.057E+13	2.037E+13	2.005E+13	1.935E+13	1.669E+13
$4d6p$	$3dkp$	2.589E+13	2.552E+13	2.527E+13	2.483E+13	2.391E+13	2.038E+13
$4d6d$	$3dkd$	4.157E+13	4.085E+13	4.035E+13	3.951E+13	3.773E+13	3.111E+13
$4d6f$	$3dkf$	4.038E+13	3.970E+13	3.923E+13	3.842E+13	3.671E+13	3.020E+13
$4f6d$	$3dkp$	1.066E+13	1.017E+13	9.847E+12	9.316E+12	8.292E+12	5.290E+12
$4f6d$	$3dkf$	3.347E+13	3.368E+13	3.379E+13	3.391E+13	3.391E+13	3.146E+13
$4f6f$	$3dkg$	7.623E+13	7.435E+13	7.305E+13	7.080E+13	6.607E+13	4.889E+13
$4f6g$	$3dkh$	5.976E+13	5.693E+13	5.505E+13	5.197E+13	4.600E+13	2.856E+13
$4f6h$	$3dkk$	1.726E+13	1.595E+13	1.512E+13	1.380E+13	1.142E+13	5.689E+12
$4d7s$	$3dks$	1.288E+13	1.265E+13	1.250E+13	1.224E+13	1.168E+13	9.556E+12
$4d7p$	$3dkp$	1.594E+13	1.565E+13	1.545E+13	1.510E+13	1.436E+13	1.156E+13
$4d7d$	$3dkd$	2.443E+13	2.388E+13	2.351E+13	2.286E+13	2.152E+13	1.660E+13
$4d7f$	$3dkf$	2.368E+13	2.314E+13	2.278E+13	2.215E+13	2.082E+13	1.591E+13
$4f7d$	$3dkf$	1.914E+13	1.936E+13	1.947E+13	1.959E+13	1.958E+13	1.733E+13
$4f7f$	$3dkg$	4.287E+13	4.162E+13	4.075E+13	3.922E+13	3.596E+13	2.430E+13
$4f7g$	$3dkh$	3.744E+13	3.531E+13	3.390E+13	3.160E+13	2.718E+13	1.495E+13
$4f7h$	$3dkk$	1.526E+13	1.390E+13	1.304E+13	1.169E+13	9.325E+12	4.040E+12
$5d5d$	$3dkd$	2.636E+13	2.581E+13	2.543E+13	2.478E+13	2.342E+13	1.828E+13
$5d5f$	$3dkf$	2.233E+13	2.212E+13	2.196E+13	2.166E+13	2.091E+13	1.717E+13
$5f5f$	$3dkg$	4.754E+13	4.584E+13	4.468E+13	4.273E+13	3.876E+13	2.564E+13
$5f5g$	$3dkh$	1.310E+13	1.246E+13	1.204E+13	1.135E+13	1.004E+13	6.215E+12
$5d6d$	$3dkd$	1.117E+13	1.087E+13	1.067E+13	1.033E+13	9.598E+12	6.887E+12
$5d6f$	$3dkf$	1.066E+13	1.049E+13	1.036E+13	1.012E+13	9.566E+12	7.094E+12
$5f6d$	$3dkf$	1.035E+13	1.029E+13	1.024E+13	1.010E+13	9.723E+12	7.484E+12
$5f6f$	$3dkg$	1.995E+13	1.909E+13	1.851E+13	1.752E+13	1.552E+13	9.117E+12
$5f7f$	$3dkg$	1.109E+13	1.058E+13	1.024E+13	9.646E+12	8.439E+12	4.635E+12
$5f7s$	$4fks$	2.128E+13	2.122E+13	2.118E+13	2.112E+13	2.097E+13	2.041E+13
$5f7p$	$4fkp$	2.444E+13	2.437E+13	2.433E+13	2.425E+13	2.408E+13	2.341E+13
$5f7d$	$4fkd$	3.005E+13	2.995E+13	2.989E+13	2.977E+13	2.953E+13	2.857E+13
$5f7f$	$4fkf$	4.241E+13	4.225E+13	4.214E+13	4.195E+13	4.154E+13	3.993E+13