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Doubly and triply excited states for different plasma sources

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Abstract. Autoionizing rates of doubly excited states as $nln'l'$ configurations with n=2-9 and n'=2-9 are calculated. Analytical expressions of decay amplitude for two-electron system are derived. Expressions for autoionizing rates with averaging over LS are obtained for many-electron systems. The n and l dependence of doubly excited states as $nln'l'$ configurations configurations are investigated.

1 Introduction

Knowledge of the basic characteristics of doubly and triply excited states is often required for solving modeling ionization phenomena in partially-ionized plasmas. These states are usually autoionizing and have a strong effect on the radiation spectrum and plasma ionization balance. Although they are sometimes omitted, autoionizing states should be included in evaluation of the equilibrium partition function for plasma LTE (local thermodynamic equilibrium). Their radiative decay is accompanied by formation of satellites to the resonance lines of ions of the next more highly charged ion and these satellites give information useful to the diagnostics of high-temperature plasma. Decay of autoionizing states can also affect population kinetics of excited levels and the radiation intensity of spectral lines.

In going from atoms to ions, a number of qualitatively new physical effects contribute to the formation of the autoionizing level spectrum. In highly charged ions as for the inner shells of heavy atoms, the role of relativistic inercombinations increases and the LS-coupling is a poor approximation. For ions of high Z the character of the spectrum changes significantly: the fine structure and hyperfine splitting increase and, in addition to dipole transitions, the higher multipoles become important. Because the autoionization decay rate is only weakly dependent on the nuclear charge Z, the rapid rise in the radiation width with Z can lead to qualitative changes in the behavior of cross-sections for various elementary processes in the vicinity of resonances.

2 Decay Amplitude

A decay amplitude [1]

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

for two-electron system could be described in the following form [2]

$$\gamma^{LS}(n_1l_1n_2l_2;n_4l_4kl_3) = (-1)^{L-(l_1-l_2+l_3-l_4)/2}\sqrt{(2l_1+1)(2l_2+1)(2l_3+1)(2l_4+1)}$$
$$\times\sqrt{\tfrac{2\pi}{k}}\eta(n_1l_1,n_2l_2)\textstyle\sum_l(-1)^l\left[P_l(n_1l_1n_2l_2;n_4l_4kl_3)\begin{Bmatrix} l_1 & l_2 & L \\ l_4 & l_3 & l \end{Bmatrix}\right.$$
$$\left.+(-1)^S P_l(n_2l_2n_1l_1;n_4l_4kl_3)\begin{Bmatrix} l_2 & l_1 & L \\ l_4 & l_3 & l \end{Bmatrix}\right] \tag{2}$$

where

$$P_l(n_1l_1n_2l_2;n_4l_4kl_3) = R_l(n_1l_1n_2l_2;n_4l_4kl_3)(-1)^{l+(l_1+l_2+l_3+l_4)/2}\begin{pmatrix} l_1 & l_3 & l \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2 & l_4 & l \\ 0 & 0 & 0 \end{pmatrix} \tag{3}$$

and $\eta(n_1l_1,n_2l_2)=1$ if $n_1l_1 \neq n_2l_2$ and $\eta(n_1l_1,n_2l_2)=1/\sqrt{2}$ if $n_1l_1 = n_2l_2$.
A radial integral for decay amplitude could be defined as

$$R_l(kl_1n_2l_2;n_4l_4n_3l_3) = \int_0^\infty r_1^2dr_1\int_0^\infty r_1^2dr_1\frac{r_<^l}{r_>^{l+1}}R_{kl_1}(r_1)R_{n_2l_2}(r_2)R_{n_4l_4}(r_2)R_{n_3l_3}(r_1) \tag{4}$$

where $R_{nl}(r)$ and $R_{kl}(r)$ are discrete and continuos hydrogenic functions. After simple, but cumbrous calculations, we can obtain for the radial integral [3]

$$R_l(kl_1n_2l_2;n_4l_4n_3l_3) = \sqrt{\tfrac{k}{1-e^{-2\pi/k}}}\frac{(2k)^{l_1}}{\sqrt{1(1+1/k^2)\cdots(l_1^2+1/k^2)}}$$
$$\times\textstyle\prod_{i=2}^4\frac{1}{(2l_i+1)}\sqrt{\frac{(n_i+l_i)!}{(n_i-l_i-1)!}}\left(\frac{2}{n_i}\right)^{l_i}\frac{2}{(n_i)^2}$$
$$\times\textstyle\sum_{m_i=0}^{n_i-l_i-1}\frac{(-1)^{m_i}}{m_i!}\frac{(2l_i+1)!(n_i-l_i-1)!}{(2l_i+1+m_i)!(n_i-l_i-1-m_i)!}\left(\frac{2}{n_i}\right)^{m_i}$$
$$\times\left(B_l^{(1)}(kl_1,n_il_im_i)+B_l^{(2)}(kl_1,n_il_im_i)\right) \tag{5}$$

where

$$B_l^{(1)}(kl_1,n_il_im_i) = \frac{(1-l+\bar{l})!(2+l+\overline{l'})!}{b^{3+l+l'}(1/n_3-ik)^{1-l+\bar{l}}}\left(\frac{1/n_3^2+k^2}{4k^2}\right)^{l_1}e^{-\frac{2}{k}arctg(kn_3)}$$
$$\times\textstyle\sum_{p=0}^{1-l+\bar{l}}\frac{1}{p!(1-l+\bar{l}-p)!}\frac{|\Gamma(l_1-n+1)|^2}{\Gamma(l_1-n+1-p)\Gamma(l_1+n+l-\bar{l}+p)}\left(\frac{1-in_3k}{1+in_3k}\right)^p \tag{6}$$

and

$$B_l^{(2)}(kl_1,n_il_im_i) = \left[\textstyle\sum_{s=0}^{2+l+\overline{l'}}\frac{(2+l+\overline{l'})!}{(2+l+\overline{l'}-s)!}-\sum_{p=0}^{1-l+\overline{l'}}\frac{(1-l+\overline{l'})!}{(1-l+\overline{l'}-s)!}\right]$$
$$\times\frac{(3+\bar{l}+\overline{l'}-s)!(-1)^{l+\overline{l'}-s}}{b^{s+1}(L-ik)^{3+\bar{l}+\overline{l'}-s}}\left(\frac{L^2+k^2}{4k^2}\right)^{l_1}e^{-\frac{2}{k}arctg(\frac{k}{L})}$$
$$\times\textstyle\sum_{p=0}^{3+\bar{l}+\overline{l'}-s}\frac{1}{p!(3+\overline{l'}+\bar{l}-s)!}\left(\frac{L-ik}{L+ik}\right)^p$$
$$\times\frac{|\Gamma(l_1-n+1)|^2}{\Gamma(l_1-n+1-p)\Gamma(l_1+n-2-\overline{l'}-\bar{l}+s+p)} \tag{7}$$

The following designations are used:

$$L = b+\frac{1}{n_3},\ b=\frac{1}{n_2}+\frac{1}{n_4},\ \bar{l}=l_1+l_3+m_3,\ \overline{l'}=l_2+l_4+m_2+m_4,\ n=\frac{1}{ik}$$

Let us demonstrate some examples.

$$R_0(ks1s;2s2s) = \frac{16}{3}\sqrt{\frac{k}{1-e^{-2\pi/k}}}\frac{3+2k^2}{(4+k^2)^4}e^{-\frac{2}{k}arctg\frac{k}{2}}$$

$$R_1(ks1s;2p2p) = \frac{16}{243}\sqrt{\frac{k}{1-e^{-2\pi/k}}}\left\{\frac{32}{(1+4k^2)}e^{-\frac{2}{k}arctg2k} - \frac{1013+432k^2+102k^4+8k^6}{(4+k^2)^4}e^{-\frac{2}{k}arctg\frac{k}{2}}\right\} \tag{8}$$

$$R_0(kp1s;2s2p) = -\frac{80}{3\sqrt{3}}\sqrt{\frac{k(1+k^2)}{1-e^{-2\pi/k}}}\frac{1}{(4+k^2)^4}e^{-\frac{2}{k}arctg\frac{k}{2}}$$

$$R_1(kp1s;2p2s) = -\frac{1024}{81\sqrt{3}}\sqrt{\frac{k(1+k^2)}{1-e^{-2\pi/k}}}\left\{\frac{1}{(1+4k^2)}e^{-\frac{2}{k}arctg2k} - \frac{811+864k^2+204k^4+16k^6}{(4+k^2)^4}e^{-\frac{2}{k}arctg\frac{k}{2}}\right\} \tag{9}$$

$$R_1(kd1s;2p2p) = -\frac{2048}{243}\sqrt{\frac{k(1+k^2)(4+k^2)}{1-e^{-2\pi/k}}}\left\{\frac{1}{(1+4k^2)^2}e^{-\frac{2}{k}arctg2k} - \frac{407+100k^2+8k^4}{128(4+k^2)^4}e^{-\frac{2}{k}arctg\frac{k}{2}}\right\} \tag{10}$$

3 Decay Amplitude for many-electron system

The matrix elements for autoionizing rate could be derived from the decay amplitude as

$$\Gamma^{LS}(n_1l_1n_2l_2;n_1'l_1'n_2'l_2'\,\|n_4l_4kl_3) = \gamma^{LS}(n_1l_1n_2l_2;n_4l_4kl_3)\gamma^{LS}(n_1'l_1'n_2'l_2';n_4l_4kl_3) \tag{11}$$

Sum over $n_4l_4kl_3[LS]$ gives us an autoionizing widths of LS term. We will not suppose to consider the mixing of configurations and $n_1l_1n_2l_2 = n_1'l_1'n_2'l_2'$ in this approximation. For this purpose the autoionizing rate could be calculated as

$$\Gamma^{LS}(n_1l_1n_2l_2\,\|n_4l_4kl_3) = \left[\gamma^{LS}(n_1l_1n_2l_2;n_4l_4kl_3)\right]^2 \tag{12}$$

For many applications, it is not important so detailed data with fixed LS. It is more convenient to use data averaging over LS. For this purpose, we have to consider the following expression:

$$A(n_1l_1n_2l_2\,\|n_4l_4kl_3) = \frac{\sum_{LS}(2L+1)(2S+1)\Gamma^{LS}(n_1l_1n_2l_2\,\|n_4l_4kl_3)}{\sum_{LS}(2L+1)(2S+1)} \tag{13}$$

The result of this averaging is [4, 5]

$$\begin{aligned} &A(n_1l_1n_2l_2;n_3l_3kl_4) \\ &= \tfrac{2\pi}{k}(2l_3+1)(2l_4+1)\sum_l\Big[\tfrac{1}{(2l+1)}P_l^2(n_1l_1n_2l_2;n_3l_3kl_4) + \tfrac{1}{(2l+1)}P_l^2(n_1l_1n_2l_2;kl_4n_3l_3) \\ &\quad -\sum_{l'}\begin{Bmatrix} l_1 & l_4 & l' \\ l_2 & l_3 & l \end{Bmatrix} P_l(n_1l_1n_2l_2;n_3l_3kl_4)P_{l'}(n_1l_1n_2l_2;kl_4n_3l_3)\Big] \end{aligned} \tag{14}$$

In the case of equivalent electrons, we obtain the following formula

$$A(n_1l_1n_1l_1;n_3l_3kl_4) = \frac{2\pi}{k}\frac{(4l_1+1)}{(2l_1+1)}(2l_3+1)(2l_4+1)\sum_l\left[\frac{2}{(2l+1)}P_l^2(n_1l_1n_2l_2;n_3l_3kl_4)\right.$$
$$\left. -\sum_{l'}\left\{\begin{array}{ccc} l_1 & l_4 & l' \\ l_1 & l_3 & l \end{array}\right\} P_l(n_1l_1n_1l_1;n_3l_3kl_4)P_{l'}(n_1l_1n_1l_1;kl_4n_3l_3)\right] \qquad (15)$$

We investigate n and l dependence of doubly excited states as $nln'l'$ configurations and triply excited states as $2snlnl'$ configurations. Even after averaging over LSJ, we obtain 8116 kinds of $A(n_1l_1n_2l_2;n_3l_3kl_4)$ and $A(n_1l_1n_1l_2;n_3l_3kl_4)$ decay amplitudes with n=2-7 and n'=2-7. Including configurations with n, n' equal to 8 and 9 give additional decay amplitudes (10,340 and 20,799 respectively) for doubly excited states. We discuss systematic features which can help to compress enormous data-set.

The probability of an autoionizing decay in a general multi-electron ion could be derived from results for two-electron system:
$(n_1l_1)^{p_1}(n_2l_2)^{p_2}(n_3l_3)^{p_3}$ and $(n_1l_1)^{p_1}(n_2l_2)^{p_2}$.
We must study two types of transitions:

$$\begin{array}{c}(n_1l_1)^{p_1}(n_2l_2)^{p_2}(n_3l_3)^{p_3} \Rightarrow (n_1l_1)^{p_1-1}(n_2l_2)^{p_2-1}(n_3l_3)^{p_3+1}k\ell \\ (n_1l_1)^{p_1}(n_2l_2)^{p_2} \Rightarrow (n_1l_1)^{p_1-2}(n_2l_2)^{p_2+1}k\ell\end{array} \qquad (16)$$

For LS averaged autoionization decay probabilities, one obtains in the two cases:

$$\begin{array}{l}\Gamma^N\left[(n_1l_1)^{p_1}(n_2l_2)^{p_2}(n_3l_3)^{p_3} \Rightarrow (n_1l_1)^{p_1-1}(n_2l_2)^{p_2-1}(n_3l_3)^{p_3+1}k\ell\right] \\ \quad = p_1p_2\left(1-\frac{p_3}{N_3}\right)A(n_1l_1n_2l_2;n_3l_3k\ell),\end{array} \qquad (17)$$

and

$$\begin{array}{l}\Gamma^N\left[(n_1l_1)^{p_1}(n_2l_2)^{p_2} \Rightarrow (n_1l_1)^{p_1-2}(n_2l_2)^{p_2+1}k\ell\right] \\ \quad = \frac{1}{2}p_1p_2\left(1-\frac{p_3}{N_3}\right)A(n_1l_1n_1l_1;n_2l_2k\ell)\end{array} \qquad (18)$$

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.

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