Autoionization of triply-excited Rydberg series

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The study of Auger spectra of multiply excited atoms and ions has been a very active area of research during the last twenty to thirty years. This observation applies particularly to doubly-excited states while more systematic studies of triply-excited states is of fairly recent origin. Studies of non-radiative decays of triply-excited states are still often limited to the lowest states although recently the first observation of Rydberg series associated with such states has been reported [1]. Most calculations have also been limited to the lowest states although this situation is beginning to change too [2,3]. In this poster we point out that the decay properties of triply-excited series can be expected to be different from the familiar behaviour of doubly-excited series.

Consider first the familiar case of doubly-excited $2lnl'$ Rydberg series in He which lie between the $n = 1$ and $n = 2$ limits. These states can only decay to the 1s limit in He II with the emission of a continuum electron with energy ϵ and angular momentum ℓ where the latter is determined by parity and angular momentum coupling selection rules. The decay rate depends on a Coulomb factor $I(2lnl',1s\epsilon\ell)$ where I stands for both direct and exchange integrals and usually comprises several R^k integrals. In addition I contains an angular factor (in practise one angular factor associated with each R^k integral) determined by the coupling conditions in the Rydberg series but if the Rydberg series is unperturbed this factor is the same for all n values and the radial integrals in I determines the decay rate as a function of n. Since the overlap between $2l$ and nl' will decrease with increasing n we expect that the decay rates will decrease with n (roughly as n^{-3}). In practise this behaviour can fairly easily be obscured for example if Rydberg series perturb each other. Nevertheless, the gradual decrease in the Auger decay rate with increasing n is a well known property of doubly-excited Rydberg series. Note that possible non-orthogonalities between initial and final state orbitals automatically are taken into account for these states in the calculation of the I factor.

Non-orthogonalities are not automatically included when we consider triply-excited states and since orthogonality simplifies the analysis we will assume that initial and final state orbitals are orthogonal. Consider a Rydberg series of the type $2s2p\,^3P\,nl\,^4L$ in a three-electron system such as Li I. This series can be considered to be built on the $2s2p\,^3P$ term in Li II and it lies above the ionization limit of Li II. This means that there are an infinity of limits of the form $1sn'l'\ ^3L$ available for the Auger decay. However, the main conclusions of the poster depends on that most of the limits are inaccessible in the approximation we have chosen. This follows

from the explicit expression for the decay rate which has three parts of which

$$I(2s2p, 1s\epsilon\ell) < nl|n'l' > \quad (1)$$

usually will be the largest and the essential point is that eq. 1 is zero unless $n = n$' and $l = l$'. Therefore in the orthogonal approximation, the Rydberg electron is a spectator electron and the decay rate is approximately the same for all values of n, being determined by the same I(2s2p,1s$\epsilon\ell$) factor since ϵ is roughly independent of n. The two other contributions are decays in which one of the $2l$ electrons is the spectator and the only limits that can be reached in these decays are therefore 1s2s ^{3}S and 1s2p ^{3}P. The I factors associated with these two decay routes, for example I(2pnl,1s$\epsilon\ell$) and I(2snl,1s$\epsilon\ell$) for the decay of 2s2pnl, *do* contain the Rydberg electron. Therefore these two contributions can be expected to be smaller than eq. 1 when $n > 2$. One practical consequence of this result is that, if the total decay rate of the lowest member of a Rydberg series has been determined, this value can serve as a first estimate for the decay rates of the higher members.

These predictions are based on a number of approximations which cannot be expected to be fulfilled very often in real atoms. Nevertheless, we have found that at least for $2l2l'nl$" series some of the predictions can be expected to be independent of the approximations and some examples have recently been established of Rydberg series in Li I which do show fairly constant Auger rates [4]. The results will be described in more detail in the poster but an example is given in table 1. In the poster we will show how some of the predictions are modified by configuration interaction and in particular by non-orthogonalities between initial and final states, while others are not.

Table 1: Total Auger decay rates (in meV) for the lowest members of the triply excited 2s2pnl ^{4}P^o series in Li I (l = s and d). Also the sum of the eigenvector components corresponding to the 2s2pnl series giving name to the term is shown (in %) in the column "purity".

2s2p(^{3}P)nl ^{4}P^o	purity	decay rate
nl=3s	93.3	9.95
3d	85.8	9.58
4s	87.0	9.62
4d	85.4	9.44
5s	86.2	9.44
5d	84.2	9.45
6s	84.8	9.44

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