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LETTER TO THE EDITOR

A formula for cancellation disappearances of atomic oscillator strengths

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Abstract. A method for prescribing the effective quantum numbers for which an oscillator strength in a Rydberg series will vanish due to cancellation effects is presented and applied to several transitions in the Cu I isoelectronic sequence.

Occasionally a specific oscillator strength in a Rydberg series is anomalously small compared with other members of the same Rydberg series and with the corresponding transition in other members of the same isoelectronic sequence. This occurs whenever the radial transition integral undergoes a change of sign along an isoelectronic sequence near values of the effective quantum numbers which correspond to a physical ion. The conditions for cancellation are very sensitive to the effective quantum numbers of the participating levels, and the anomaly is usually very sharp, restricted to a single Rydberg transition and a single member of the isoelectronic sequence. An example of such cancellation effects is shown in figure 1, for the $4p\ ^2P_{3/2}$–$5d\ ^2D_{5/2}$ transition in the Cu I isoelectronic sequence. Here the oscillator strength (computed using the numerical Coulomb approximation by A Lindgård 1978, private communication) for Kr VIII is diminished by more than four orders of magnitude from those of neighbouring ions, Br VII and Rb IX. This oscillator strength cancellation is not a unique phenomenon, but, on the contrary, has many possibilities for occurrence which can be systematically examined by the methods to be described below.

A knowledge of the occurrence of anomalously small oscillator strengths can be valuable for a number of reasons. It can be utilised in term analysis studies, since it explains the absence of lines which would otherwise be expected to be present (e.g., the 3s–4p resonance lines in Mg II are anomalously weak compared to other members of the Na I isoelectronic sequence because of such a cancellation). Anomalously low oscillator strengths in low lying resonance transitions can be useful for astrophysical abundance determinations, since they are unsaturated in absorption spectra and thus permit lineshape studies. Knowledge that a normally strong transition becomes insignificant for a specific ion is also valuable in atomic lifetime measurements which incorporate cascade information into the analysis. The method described here utilises effective quantum numbers, and thus permits the use of quantum defect extrapolations to make predictions in the nature of a simple yes or no statement about the disappearance of the oscillator strength. This method also

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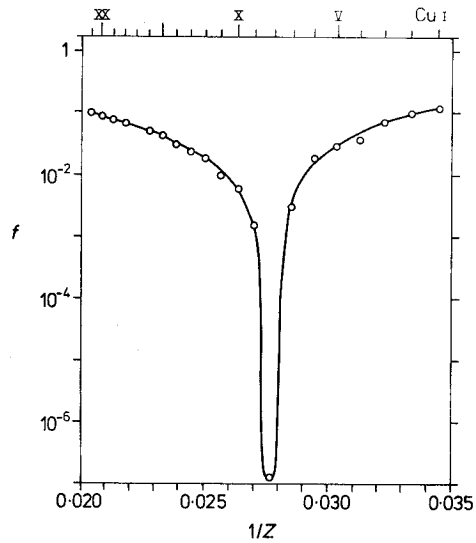

Figure 1. Absorption oscillator strength versus reciprocal nuclear charge for the $4p\ ^2P_{3/2}$–$5d\ ^2D_{5/2}$ transition in the Cu I isoelectronic sequence.

provides a quick test of the presence of this cancellation for any transition for which effective quantum numbers are known.

Rydberg series are common to the spectra of many atoms. Within such a series the term values E_{nl} of a level of principal and angular momentum quantum numbers n and l can be specified by an extended Ritz formula (Edlén 1964) giving the quantum defects δ_{nl} as a power series in the reduced energy $\epsilon_{nl} = E_{nl}/R\zeta^2 = -1/n_l^{*2}$ (here R is the Rydberg energy, ζ the core charge and $n_l^* = n - \delta_{nl}$ is the effective principal quantum number). When δ_{nl} varies slowly with ϵ_{nl}, the one-electron model and hence the quantum defect method are valid approximations. Using the quantum defect method, Burgess and Seaton (1960) have derived a simple analytic approximation for the partial cross section for photoionisation. Their results are equivalent to the well known tables of Bates and Damgaard (1949), but have some advantages in that they combine slowly varying tabulated parameters with simple analytic functions.

It is easy to apply the photoionisation formula of Burgess and Seaton (1960) to the discrete spectrum, using the concept of an oscillator strength distribution in energy which is analytic across the ionisation limit (Fano and Cooper 1968, Seaton 1958). The result is

$$n_l^{*3} f_{nl,n'l'} = A \cos^2\pi(n_{l'}^* - n_l^* - \chi) \tag{1}$$

where $f_{nl,n'l'}$ is the absorption oscillator strength for a lower level nl and an upper level $n'l'$, and A and χ are slowly varying functions of the effective quantum numbers for given l and l'. The functions A and χ can be evaluated numerically from tables given by Burgess and Seaton (1960). This approach has been used by Gruzdev to compute a number of oscillator strengths (Gruzdev 1966, 1967a, b, Gruzdev and Prokofev 1966); Gruzdev (1967a) contains a more explicit version of our equation (1).

The cancellation effects in the radial transition integral which we are studying manifest themselves directly in equation (1) through the zeros of the cosine, which

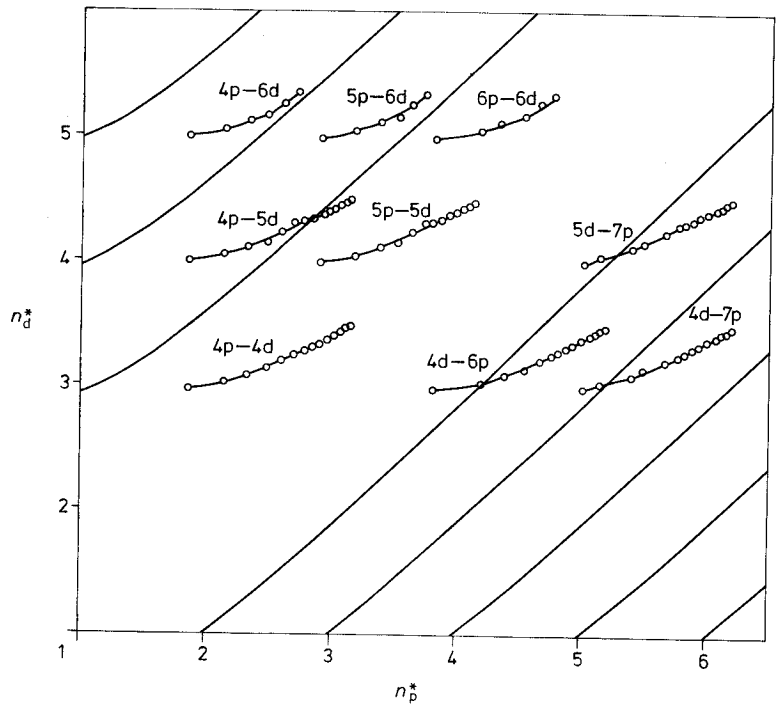

Figure 2. Plot of the effective quantum numbers along the Cu I isoelectronic sequence for various Rydberg transitions, along with the lines of vanishing oscillator strength predicted by equation (1).

occur whenever $n_{l'}^* - n_l^* - \chi = k + \frac{1}{2}$, where k is an arbitrary integer. Using expressions given by Burgess and Seaton (1960) for χ, the conditions for cancellation for $n_l^* > l + 1$ become

$$n_{l'}^* = n_l^* + k + \tfrac{1}{2} + a_{ll'} + b_{ll'}/n_l^* + c_{ll'}/n_l^{*2} - \alpha_{ll'}/(n_{l'}^{*2}/n_l^* - 1) - \beta_{ll'}/(n_{l'}^{*2}/n_l^{*2} - 1) \quad (2)$$

where the quantities $a_{ll'}$, $b_{ll'}$, $c_{ll'}$, $\alpha_{ll'}$ and $\beta_{ll'}$ are simple numerical coefficients, which are given in table 3 of the paper by Burgess and Seaton (1960). (For smaller n_l^* tables 6–8 may be used instead for greater precision.) The formal solution of equation (2) requires extraction of the roots of polynomial equations of up to sixth order. However, for values of k such that $n_{l'}^*$ and n_l^* are not too close together (in which case the oscillator strengths and transition probabilities become small due to the wavelength dependence), the appropriate root can be obtained by choosing a value for $n_{l'}^*$ and iterating equation (2) for successively better approximations for $n_{l'}^*$.

With this single physical root, equation (2) represents a family of curves (approaching parallel straight lines with a 45° slope for large quantum numbers) on a plot of $n_{l'}^*$ versus n_l^*. It should be noted that the formulation of Burgess and Seaton is approximate in that it is not symmetric under interchange of upper and lower level quantum numbers, so values of $n_{l'}^* < n_l^*$ should be obtained by interchanging l and l' in equation (2), and *not* by allowing k to take on negative values. A confrontation with experimental results can be obtained by plotting the corresponding $n_{l'}^*$ and n_l^* values for given Rydberg transitions along an isoelectronic sequence, and

looking for coincidences or near coincidences between the experimental points and the lines of nodes predicted by equation (2).

A plot of n_d^* versus n_p^* for a number of levels in the Cu I sequence is given in figure 2, along with the nodes predicted by equation (2). The circles represent, from left to right, Cu I to Mo XIV for all plots except *n*p–6d, which extend only from Cu I to Se VI. Existing term value data have been supplemented by Ritz formula quantum defect extrapolations for the 6d and 7p levels. Notice that there is a coincidence with a node line for the 4p–5d transition at Kr VIII, corresponding to the cancellation effects depicted in figure 1, as well as another coincidence for the 4d–6p transition at Zn II. Calculations using the numerical Coulomb approximation (A Lindgård 1978, private communication) indicate that the oscillator strength for the 4d $^2D_{5/2}$–6p $^2P_{3/2}$ transition for Zn II is diminished by more than three orders of magnitude from that in Ga III, and by over four orders of magnitude from that in Cu I.

Thus a comparison of lines of vanishing oscillator strength given by equation (2) can be made with the effective quantum numbers of any physical state, determined either directly experimentally, or by Ritz formula extrapolations. This provides a method for testing any specific transition for cancellation effects, or for conducting a systematic search for systems which exhibit these cancellation effects.

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