CALCULATIONS AT SERIES LIMITS IN ONE-ELECTRON SYSTEMS

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Introduction

The behavior of atoms in high quantum levels is generally well understood—in principle. For sufficiently large values of the principle quantum number, discrete levels that would exist for an isolated atom, do not. They are said to be dissolved, or quenched by perturbations from surrounding atoms and ions. In practice, the calculation of relevant atomic properties can become quite involved, especially if one strives for accuracy. Detailed references may be found in the papers by Stehlé and Jacquemot, Hummer and Mihalas, or the book by Griem.

We draw attention here to a general principle that should be of practical value in the calculation of opacity near the series limits. We show that as soon as the Lyman or Balmer lines overlap and the individual profiles wash out, the net absorption cross section rapidly approaches the value at the series limit. It has been known for more than seventy years that the line and continuous opacities merge smoothly. We are unaware of a discussion of the rapidity of this convergence, which has a practical value for the calculation of opacity.

Independent of the difficult question of the relative contributions of line and continuous opacity, we can get a good estimate of their sum. The accuracies of estimates for two series are discussed below. We offer the following thoughts as a computational aid. They may also be of heuristic value.

A Mean Line Absorption Cross Section

Let us begin by considering the line opacity in a series. We take the Lyman series for simplicity. For lines with wavenumbers greater than that of $L_\alpha$, we may define a mean cross section for the line $L_n$ in the following way. Associate an interval, $\Delta \tilde{\nu}_n$ cm$^{-1}$, with each line that extends halfway to the neighbors on either side. With the Rydberg formula, we have

$$\Delta \tilde{\nu}_n = \frac{1}{2}[\tilde{\nu}_{n+1} + \tilde{\nu}_n] - \frac{1}{2}[\tilde{\nu}_n + \tilde{\nu}_{n-1}] = \left[ \frac{2n \cdot Ry}{(n - 1)^2 \cdot (n + 1)^2} \right].$$

Equation (1)

Clearly, $\Delta \tilde{\nu}_n$ represents the interval most logically associated with an individual line in the series. We can use it to define a mean line photoabsorption cross section $< \sigma_n >$, such that

$$< \sigma_n > \cdot \Delta \tilde{\nu}_n = \frac{\pi e^2}{\mu c^2} f_{mn}.$$ 

Equation (2)
Table 1: Mean Cross Sections (Power of ten shown in parentheses)

| n(upper) | Lyman          | Balmer         |
|----------|----------------|----------------|
|          | f-value        | < σ<sub>n</sub> > cm<sup>2</sup> | f-value        | < σ<sub>n</sub> > cm<sup>2</sup> |
| 10       | 1.60537(-3)    | 6.35353(-18)   | 3.85061(-3)    | 1.52395(-17)   |
| 15       | 4.68624(-3)    | 6.32994(-18)   | 1.07022(-3)    | 1.44560(-17)   |
| 20       | 1.96675(-4)    | 6.32172(-18)   | 4.41644(-4)    | 1.41958(-17)   |
| 25       | 1.00456(-4)    | 6.31796(-18)   | 2.23836(-4)    | 1.40776(-17)   |
| 30       | 5.80583(-4)    | 6.31587(-18)   | 1.28882(-4)    | 1.40141(-17)   |
| 60       | 7.24117(-6)    | 6.31236(-18)   | 1.59530(-5)    | 1.39067(-17)   |
| ∞        | 6.31119(-18)   | 1.38712(-17)   |

The symbols e and c have their usual meanings. Here, μ = m<sub>e</sub>/(1 + m<sub>e</sub>/m<sub>p</sub>) is the reduced mass, which we must use to obtain the desired accuracy below. Values of the physical constants were taken from the NIST website. We use e(esu) = e(SI)∗c/10, a<sub>H</sub> = a<sub>0</sub>/(1 + m<sub>e</sub>/m<sub>p</sub>), and Ry = e<sup>2</sup>/(2a<sub>H</sub>hc).

There would be a factor of λ<sup>2</sup> on the right of Equation (2) had we used wavelengths rather than wavenumbers to define the interval associated with the n<sup>th</sup> series member.

Oscillator strengths for the Lyman lines have a simple closed form (cf. Bethe and Salpeter p. 263):

\[
f_{1s,np} = \frac{2^8 n^5 (n-1)^2 n-4}{3(n+1)^2 n+4},
\]

which was used to derive the entries in column 2, of Table 1, which extend somewhat beyond the tabulation of Green, Rush, and Chandler. The last two figures given in this reference and in our Table 1 are of heuristic and illustrative value only, since relativistic effects are of the order of (1/137)<sup>2</sup> and apply to the real atom. We have used non-relativistic formulae throughout. The last entry gives the continuous absorption cross section calculated at the Lyman series limit. The corresponding gaunt factor is 0.797301. Karzas and Latter gave 0.7973.

Even for L<sub>10</sub>, <σ<sub>10</sub>> differs from the cross section at the series limit by less than one per cent. Calculations for the Balmer series show a similar convergence to the series limit, 1.387·10<sup>-17</sup> cm<sup>2</sup> though less rapid. The error at H<sub>10</sub> is nearly 10%. This is entirely consistent with the beautiful experimental work of Wiese and coworkers which shows a drop in the intensity of about 10% between λ3700 (essentially, H<sub>10</sub>) and the Balmer limit.

By H<sub>20</sub>, the difference is only 2%. This line (λ<sub>air</sub>3682.81) is still 36.83Å from the series limit, λ<sub>air</sub>3645.98, and anyone who analyzes lines in this region needs to have the H I opacity accurately calculated. For conditions in the mean solar photosphere, the Balmer lines overlap and flatten near the position of H<sub>20</sub>, so the total opacity should be within 2% of that at the series limit from this point.
Calculations of the opacity near the Balmer and Lyman limits are therefore not sensitive to the difficult questions involving the “existence” of high upper levels. Whatever the relative proportions of line and continuous opacity, the sum must approach the value at the head of the series.

The rigorous approach to calculations in this region is described for example, by Stehlé and Jacquemot and in elegant detail, by Seaton, who also treats the non-hydrogenic case. At each wavelength, some fraction of the opacity is calculated as line opacity, and the complement is calculated as continuous absorption. The recipe for the division follows from the probability that a given level \( n \) will exist. This probability is given in the references already cited, and can be somewhat tedious. It is therefore well for anyone coding this problem anew to be aware that the total opacity must merge rapidly to that at the series limit. We have shown that this must be so for the Lyman and Balmer series. Higher series should be investigated. If the convergence to the series limit is not rapid, the ideas outlined here will require modification to be useful computationally.

**A Proof**

We sketch a proof of the result that the quotient \( \frac{f_{mn}}{\Delta \nu_n} \) reaches a limit for large \( n \) that is independent of \( n \), and which converges to the continuous absorption cross section at the series limit. It is only necessary to divide the \( f \)-value given by Equation (3) by \( \Delta \nu \), which appears on the right of Equation (1), and take the limit as \( n \) approaches infinity. We can then readily show that

\[
\sigma_{\text{lim}} = \lim_{n \to \infty} \frac{\pi e^2}{\mu c^2} \cdot \frac{f_{1s, np}}{\Delta \nu} = \pi e^2 \cdot 27 \exp(-4) \cdot \frac{1}{3\text{Ry}}.
\]

If we work out the cross section from first principles, we have

\[
\sigma_{\text{lim}} = \frac{8\pi^3 \nu}{3c^3 a_H^3} \cdot | < 1, s|E = 0, p > |^2.
\]

The dimensionless matrix element for a freed electron with zero energy has the absolute numerical value 2.165364. Both Equations (4) and (5) agree for the cross section for the series limit given in Table 1, as they must.

We omit details of a corresponding proof that we have carried out for the Balmer series. It is necessary to convert the closed-form expressions for the relevant radial integrals (cf. Bethe and Salpeter, Eqs. 63.4) to \( f \)-values, and perform an average for the \( 2s - np, 2p - nd \), and \( 2p - ns \) series:

\[
< \sigma_{2-n} > = \frac{1}{4} [\sigma_{2s-np} + 3\sigma_{2p-nd} + 3\sigma_{2p-ns}].
\]

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