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Comment on coefficients of fractional parentage of the form $(l^{2l+1}|\}l^{2l+2})$

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For the special case of half-filled subshells, Racah showed in 1943 that his formula relating the coefficients of fractional parentage for a given particle configuration to those for the corresponding hole configuration requires an additional phase factor $(-1)^{(v-1)/2}$, where v is the seniority of the half-filled configuration. This phase factor is incorrectly printed in Racah's 1943 paper as $(-1)^{v-1/2}$. Furthermore, this phase factor is omitted in the 1952 paper by Rosenzweig, resulting in sign errors in the table of $(d^5|\}d^6)$ coefficients. These rather old errors have often been repeated in subsequent publications, including even some recently published monographs and textbooks.

The coefficients of fractional parentage (CFP) for configurations having a more than half-filled subshell are usually calculated in terms of those for the corresponding less than half-filled subshell with the use of the following formula first derived by Racah[1]:

$$(l^{4l+1-n}\alpha SL\,|\}l^{4l+2-n}\alpha'S'L') = (-1)^{S+S'+L+L'-l-1/2}\left[\frac{(n+1)(2S+1)(2L+1)}{(4l+2-n)(2S'+1)(2L'+1)}\right](l^n\alpha'S'L'|\}l^{n+1}\alpha SL)\ . \quad (1)$$

Racah points out (cf. Ref. 1, end of Sec. 4) that Eq. (1) is correct only up to a phase in the case $n=2l$, i.e., for the CFP of the configuration l^{2l+2}. This phase arises from the symmetry of the particle and hole configurations l^{2l+1} for the half-filled subshell.[2] Racah found [cf. Eq. (65) of Ref. 1] that this phase factor depends on the seniority quantum number v of the half-filled configuration l^{2l+1}. Note that this phase is necessary even for p subshells, for which the seniority quantum number is usually superfluous. Specifically, this phase factor is $(-1)^{(v-1)/2}$, although it is incorrectly printed in Eq. (65) of Ref. 1 as $(-1)^{v-1/2}$. For the case $n=2l$, then, the right side of Eq. (1) must be multipled by $(-1)^{(v-1)/2}$.

Rosenzweig[3] has published tables of CFP for almost filled d subshells. He used Racah's formula to obtain these CFP [cf. Eq. (23) of Ref. 3], but he omits the phase factor $(-1)^{(v-1)/2}$ in computing the coefficients $(d^5vLS|\}d^6v'L'S')$. Thus the values for these CFP in his Table VI are in error by this phase, i.e., whenever $v=3$ for a term of the d^5 configuration, the CFP should be multiplied by -1.

Far from being of only historical interest, these errors concerning Racah's phase factor have been repeated in a number of more recent publications. Thus the monograph by Nielson and Koster[4] includes Racah's phase, but gives the misprinted form $(-1)^{v-1/2}$ originally appearing in Eq. (65) of Ref. 1. Several[5-7] recent textbooks on atomic physics reproduce Racah's formula (1) above but fail to mention the necessity for the additional phase factor when $n=2l$. One of these books[5] reproduces the erroneous table of Rosenzweig[3] for the $(d^5vLS|\}d^6v'L'S')$ CFP and also has an erroneous sign for the $(p^3v=3^2D|\}p^4v=2^1D)$ CFP. [These errors occur in Table 20, p. 105 and Table 25, pp. 108–109 of Ref. 5(a), and in Tables 5.3 and 5.8 of Ref. 5(b).] The sign errors in Ref. 5(b) have already been noted by Reader.[8]

Users of tables of CFP can easily check for themselves whether Racah's phase factor has been properly taken into account. One need only verify that the ratio of the coefficients $(l^{2l+1}vLS|\}l^{2l+2}v'L'S')$ and $(l^{2l}v'L'S'|\}l^{2l+1}vLS)$ has the sign $(-1)^x$, where

$$x=(v-1)/2+L+S+L'+S'-l-1/2\ . \quad (2)$$

Among those works which give CFP tables for more than half-filled subshells and which this author has checked, Racah's phase is properly taken into account in the books by Shore and Menzel[9] and by Cowan[10] and also in the CFP computer programs of Allison[11] and of Chivers.[12]

Needless to say, sign errors in CFP can lead to significant errors in numerical atomic-physics calculations. Of the author's published works, none is affected by this phase error, although some recent unpublished results have had to be recalculated. The seeming ignorance of the Racah phase factor in several recently published text books[5-7] (Cowan's book is a notable exception; cf. pp. 263–265 of Ref. 10) has motivated the author to publicize the matter in this Comment in order to limit the wider propagation of this ignorance and its possible effect on future calculations.

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