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Magnetic Interactions in Mixed Configurations

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Magnetic interactions for mixed atomic configurations are given in tensor notation. These results are obtained by expanding in powers of (v/c^2) the equivalent operators for the Breit equation. An operator is obtained which has angular dependence unlike that of any operator appearing in the equivalent electron case. The particular case of interactions within configuration $l^n\, l'^m$ is discussed.

I. INTRODUCTION

Conventional theoretical analysis of atomic spectra involves fitting of the observed energy levels with Slater and spin-orbit parameters, as well as parameters arising from perturbations caused by other configurations. Recent work,[1,2] however, has indicated the desirability of also considering the effects of two-body magnetic interactions such as spin-spin and spin-other-orbit.

The Hamiltonians for the magnetic interactions have been considered by many authors[3] for configurations l^n, but little attention has been directed to work in the mixed configuration case.[4,5] Recent work[6] demonstrated how the magnetic interactions for the configuration l^n could be obtained in a straightforward manner starting from the Breit equation by use of the equivalent operator formalism. We have utilized this formalism to obtain the magnetic interactions for the mixed configuration case. The results are completely general and can also be applied to the interaction of one configuration with another.

II. METHODS AND RESULTS

An equivalent operator is defined such that its matrix element taken between nonrelativisitic wave functions produces the same result as does the relativistic operator evaluated between relativistic states. This allows calculations to be carried out in the nonrelativistic scheme, where the powerful tensor techniques of Racah[7] can be more fully exploited. The equivalent operator for the Breit interaction is obtained by treating the Breit interaction as a perturbation to the Dirac Hamiltonian. This equivalent operator has been obtained in form valid for mixed configurations in a previous paper[8]; the results are rather complicated and therfore will not be repeated here. These previous results contain products of n-j symbols,

radical integrals involving the large (F) and small (G) components of the relativistic radial wave function and tensor operators for mixed configurations $\vec{W}^{(\kappa k)K}(l_1, l_2)$. These tensor operators are defined by the equations[9]

$$\vec{W}^{(\kappa k)K}(l_1, l_2) = \sum_i \vec{w}_i{}^{(\kappa k)K}(l_1, l_2)\langle \tfrac{1}{2} l_3 || w^{(\kappa k)}(l_1, l_2) || \tfrac{1}{2} l_4\rangle = [\kappa, k]^{1/2}\delta(l_1, l_3)\delta(l_2, l_4). \tag{1}$$

In order to obtain the magnetic interactions, we expand in powers of $(v/c)^2$ the results given in Eqs. (16)–(21) of REFS; the lowest nonvanishing terms give the desired interactions. The procedure followed[6] consists of expanding the radial terms in powers of $(v/c)^2$, and then carrying out the summations which appear in the results of REFS. To first order in $(v/c)^2$, the large component F_j becomes just the nonrelativistic wave function R_l; the small component G_j is related, in this order, to F_j by the equation

$$G_j = (\hbar/2mc)(d/dr - \kappa/r)F_j\,, \quad \text{where} \quad \kappa = (-1)^{j+l-\frac{1}{2}}[j]/2. \tag{2}$$

Three radial parameters appear often in our results

$$P^K(l_a l_b; l_c l_d) = (e\hbar/2mc)^2 \iint_{r_2>r_1} R_{la}(r_1)R_{lc}(r_1)R_{lb}(r_2)R_{ld}(r_2)(r_1{}^K/r_2{}^{K+3})dr_1 dr_2. \tag{3}$$

$$Q^K(l_a l_c; l_b l_a) = (e\hbar/2mc)^2 \iint r_1 R_{la}(r_1)R_{lb}(r_1)(r_<{}^K/r_>{}^{K+3})[R_{lc}(r_2)(d/dr_2)R_{ld}(r_2) - R_{ld}(r_2)(d/dr_2)R_{lc}(r_2)]\,dr_1 dr_2$$

and R^K of Marvin[4]

$$R^K(l_a l_b; l_c l_d) = \tfrac{1}{2}(e\hbar/2mc)^2 \iint R_{la}(r_1)R_{lc}(r_1)R_{lb}(r_2)R_{ld}(r_2)(r_<{}^K/r_>{}^{K+3})dr_1 dr_2. \tag{4}$$

If $l_a = l_b$ and $l_c = l_d$ (or $l_a = l_d$ and $l_c = l_b$), $P^K = R^K$. Following the procedure outlined above, we obtain the following results:

A. Spin-Spin Term

$$2\sqrt{5}\sum \begin{Bmatrix} 1 & 1 & 2 \\ K+2 & K & K+1 \end{Bmatrix}[(K+1)(K+2)(2K+3)]^{1/2}\langle l_a || C^{K+2} || l_b\rangle\langle l_c || C^K || l_d\rangle \times P^K(l_a l_c; l_b l_d)\vec{w}_i{}^{(1K+2)K+1}(l_a, l_b)\cdot\vec{w}_j{}^{(1K)K+1}(l_c, l_d), \tag{5}$$

where the sum is over K, l_a, l_b, l_c, l_d, and over $i \neq j$.

B. Orbit-Orbit Term

$$-8\sum(2K+1)/(K+2)\langle l_a || C^K || l_b\rangle\langle l_c || C^K || l_d\rangle[(l_b)(l_b+1)(2l_b+1)(l_d)(l_d+1)(2l_d+1)]^{1/2} \times \begin{Bmatrix} K & K+1 & 1 \\ l_a & l_a & l_b \end{Bmatrix}\begin{Bmatrix} K & K+1 & 1 \\ l_c & l_c & l_d \end{Bmatrix} R^K(l_a, l_c; l_b l_d)\vec{w}_i{}^{(0K+1)K+1}(l_a, l_b)\cdot\vec{w}_j{}^{(0K+1)K+1}(l_c, l_d)\,, \tag{6}$$

where the sum is over K, l_a, l_b, l_c, l_d, and $i \neq j$.

C. Spin-Spin Contact Term

$$-\sum\Big\{2[(K+1)(K+2)]^{\frac{1}{2}}[K+1]^{-\frac{1}{2}}\langle l_a || C^K || l_b\rangle\langle l_c || C^{K+2} || l_d\rangle\vec{w}_i{}^{(1K)K+1}(l_a, l_b)\cdot\vec{w}_j{}^{(1K+2)K+1}(l_c, l_d)$$
$$+(K+2)/(2K+3)\langle l_a || C^K || l_b\rangle\langle l_c || C^K || l_d\rangle\vec{w}_i{}^{(1K)K+1}(l_a, l_b)\cdot\vec{w}_j{}^{(1K)K+1}(l_c, l_d)$$
$$+(K-1)/(2K-1)\langle l_a || C^K || l_b\rangle\langle l_c || C^K || l_d\rangle\vec{w}_i{}^{(1K)K-1}(l_a, l_b)\cdot\vec{w}_j{}^{(1K)K-1}(l_c, l_d)$$
$$-\langle l_a || C^K || l_b\rangle\langle l_c || C^K || l_d\rangle\vec{w}_i{}^{(1K)K}(l_a, l_b)\cdot\vec{w}_j{}^{(1K)K}(l_c, l_d)\Big\}\,(e\hbar/2mc)^2\int(R_{la}R_{lb}R_{lc}R_{ld}/r^2)dr, \tag{7}$$

where the sum is over K, l_a, l_b, l_c, l_d, and $i \neq j$. As in the one-configuration case,[6] the spin-spin contact term can be written

$$(2\mu_0^2/3r^2)\sum\delta(r_i - r_j)(-1)^{K+\beta}\langle l_a \| C^K \| l_b\rangle\langle l_c \| C^K \| l_d\rangle \vec{w}_i^{(1K)\beta}(l_a, l_b)\cdot \vec{w}_j^{(1K)\beta}(l_c, l_d) - (16\pi/3)\mu_0^2\delta(\vec{r}_1 - \vec{r}_2)\left[\vec{s}_1\cdot\vec{s}_2 - 3(\vec{s}_1\cdot\vec{r})(\vec{s}_2\cdot\vec{r})/r^2\right]; \quad (3)$$

The sum above is over K, β, and $i \neq j$. The matrix elements of the second term above can easily be shown to be zero when evaluated between any two particle states $\langle l_1 l_2 SL \mid$ and $\mid l_3 l_4 S\bar{L}\rangle$, so that the spin-spin contact term is just given by the first term in Eq. (8).

D. Spin-other-Orbit Term

$$\sum[K+1]^{-\frac{1}{2}}\left[\left(\frac{(l_d+l_c+K+2)(l_d+l_c-K)[(K+1)^2-(l_c-l_d)^2]}{K+1}\right)^{1/2}\langle l_a \| C^{K+1} \| l_b\rangle\langle l_c \| C^{K+1} \| l_d\rangle\right.$$

$$\times P^{K-1}(l_a l_c; l_b l_d) - 2\left(\frac{(l_a+l_b+K+2)(l_a+l_b-K)[(K+1)^2-(l_a-l_b)^2]}{K+1}\right)^{1/2}$$

$$\left.\times\langle l_a \| C^K \| l_b\rangle\langle l_c \| C^K \| l_d\rangle P^K(l_a l_c; l_b l_d)\right]\vec{w}_i^{(0K+1)K+1}(l_a, l_b)\cdot\vec{w}_j^{(1K)K+1}(l_c, l_d)$$

$$+[K]^{-\frac{1}{2}}\left[\left(\frac{(l_c+l_d+K+2)(l_c+l_d-K)[(K+1)^2-(l_d-l_c)^2]}{K+1}\right)^{1/2}\langle l_a \| C^K \| l_b\rangle\langle l_c \| C^K \| l_d\rangle P^K(l_c l_a; l_d l_b)\right.$$

$$\left.-2\left(\frac{(l_a+l_b+K+2)(l_a+l_b-K)[(K+1)^2-(l_a-l_b)^2]}{K+1}\right)^{1/2}\langle l_a \| C^{K+1} \| l_b\rangle\langle l_c \| C^{K+1} \| l_d\rangle P^{K-1}(l_c l_a; l_d l_b)\right]$$

$$\times\vec{w}_i^{(0K)K}(l_a, l_b)\cdot\vec{w}_j^{(1K+1)K}(l_c, l_d)$$

$$+[K]^{-1}[K(K+1)]^{1/2}\langle l_a \| C^K \| l_b\rangle\langle l_c \| C^K \| l_d\rangle\{-2[l_d(l_d+1)-l_c(l_c+1)][K^{-1}P^{K-2}(l_a l_c; l_b l_d)$$

$$-(K+1)^{-1}P^K(l_c l_a; l_d l_b)] + [l_b(l_b+1)-l_a(l_a+1)]$$

$$\times[K^{-1}P^{K-2}(l_a l_c; l_b l_d) - (K+1)^{-1}P^K(l_c l_a; l_d l_b)] - 2Q^{K-1}(l_a l_c; l_b l_d) + Q^{K-1}(l_c l_a; l_d l_b)\} \quad (9)$$

$$\times\vec{w}_i^{(0K)K}(l_a, l_b)\cdot\vec{w}_j^{(1K)K}(l_c, l_d),$$

where the sum is over K, l_a, l_b, l_c, l_d, and $i \neq j$.

III. SPECIALIZATION TO THE CONFIGURATION $l^n l'^m$

The previous results are valid for the general case, and can be used, for example, to investigate the perturbation due to the magnetic interactions of one configuration by another. This effect is considered by some to be quite important.[10] Another important field of application of these results, however, is that of the effect of the magnetic interactions within a configuration $l^n l'^m$.

In the case of an $l^n l'^m$ configuration, the interactions should be expressed, whenever possible, in terms of the operators[11]

$$\vec{w}^{\pm(\kappa k)}(l, l') = 2^{-\frac{1}{2}}[\vec{w}^{(\kappa k)}(l, l') \pm (-1)^{\kappa+k}\vec{w}^{(\kappa k)}(l', l)],$$

as these operators have definite transformation properties with respect to the groups $Sp_4(l+l'+1)$ and $R_2(l+l'+1)$.

The operators corresponding to the interaction of two equivalent electrons are given in Ref. 6; we are concerned here only with the terms corresponding to the interaction of inequivalent electrons. We have seen in the previous section that in the spin-spin and spin–other-orbit interactions our results do not contain Marvin's integrals. It is interesting, however, to introduce these integrals at this point by the relations

$\frac{1}{2}[P^K(ll';l'l)+P^K(l'l;ll')]=M^K$ and $P^K(ll';ll')=N^K$.

We further separate the Hamiltonians for the various interactions into $\mathcal{H}^a$ and $\mathcal{H}^s$, which are, respectively, antisymmetric and symmetric with respect to interchange of l and l' in the angular portion. For example, we can write for the spin-spin part:

$$\mathcal{H}_{ss}^{\ s}=2\sqrt{5}\sum_{K,\,i\neq j}\begin{Bmatrix}1&1&2\\K+2&K&K+1\end{Bmatrix}[(K+1)(K+2)(2K+3)]^{\frac{1}{2}}M^K\{\langle l\|C^{K+2}\|l\rangle\langle l'\|C^K\|l'\rangle$$

$$\times[\vec{w}_i(1K+2)K+1(l,l)\cdot\vec{w}_j(1K)K+1(l',l')]+\langle l\|C^K\|l\rangle\langle l'\|C^{K+2}\|l'\rangle[\vec{w}_i(1K+2)K+1(l',l')\cdot\vec{w}_j(1K)K+1(l,l)]\}$$

$$+2N^K\langle l\|C^K\|l'\rangle\langle l\|C^{K+2}\|l'\rangle[\vec{w}_i-(1K+2)K+1(ll')\cdot\vec{w}_j-(1K)K+1(l,l')]$$

and

$$\mathcal{H}_{ss}^{\ a}=5^{\frac{1}{2}}\sum_{K,\,i\neq j}\begin{Bmatrix}1&1&2\\K+2&K&K+1\end{Bmatrix}[(K+1)(K+2)(2K+3)]^{\frac{1}{2}}[P^K(ll';l'l)-P^K(l'l;ll')]\{\langle l\|C^{K+2}\|l\rangle\langle l'\|C^K\|l'\rangle$$

$$\times[\vec{w}_i(1K+2)K+1(l,l)\cdot\vec{w}_j(1K)K+1(l',l')]-\langle l\|C^K\|l\rangle\langle l'\|C^{K+2}\|l'\rangle[\vec{w}_i(1K+2)K+1(l',l')\cdot\vec{w}_j(1K)K+1(l,l)]\}\ .$$

We have verified that for the configuration dp, the symmetric parts of the spin-spin and spin–other-orbit Hamiltonians are identical to $\mathcal{H}_M^{II}$ and $\mathcal{H}_M^{I}$ of Marvin.[4]

If one neglects the orbit-orbit interaction, which is absorbed by the effective Hamiltonian produced by configuration interaction, and the spin-spin contact term, which is absorbed by the Coulomb interaction, one finds that the total number of parameters required to represent the magnetic interactions within the configuration $l^ml'^m$ is $4l_<+2$, where $l_<$ is the smaller of l and l'. This number is small enough to permit a fit of these parameters in numerous spectra (for example, the configurations d^np of the third spectra of the iron group).

IV. DISCUSSION

We have expanded the equivalent operator form of the Breit equation in powers of $(v/c)^2$ in order to obtain the magnetic interactions in a tensorial form valid for mixed configurations. The results obtained to order $(v/c)^2$ are given in Sec. II; all two-body terms (except those having the angular dependence of the Coulomb interaction) having angular dependence different from those given in Sec. II are zero to order $(v/c)^2$.

There are two very interesting points to be made concerning the results of Sec. II. First, Marvin's integrals do not represent all of the radial parameters arising from the magnetic interactions. Because of the differences in methods of derivation, it is not at all clear why our results differ from those of Marvin.[4] We note, however, that a recent paper[5] which considered specific cases of magnetic interaction in mixed configurations also obtained integrals such as P^K and Q^K. The second point of interest is that an operator has been found in Sec. II. D which has an angular dependence not found in the equivalent electron case. The assignment of the new operator to the spin–other-orbit interaction is somewhat arbitrary. The general form of the angular dependence is certainly analogous to that of the other spin–other-orbit interactions, but the method of derivation does not actually give any indication as to which (if any) of the classical operators would give rise to such a term. Application of these results to term analysis in configurations $l^Nl'^M$ would appear to be straightforward. As shown in Sec. III, the number of additional radial parameters introduced by the magnetic interactions in such cases is not prohibitive. However, analyses which entail decomposing the interactions into parts having well-defined symmetry properties[7,11,12] will require that the results of Sec. II be restated in terms of the angular operators $w^{\pm}(\kappa K)$. This is not difficult to do, but the resulting expressions are considerably less concise than the results given in Eqs. (6)–(10).

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Self-Broadening of Cesium Resonance Lines at 8521 and 8944 Å*

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Absorption profiles of cesium resonance lines at 8521 and 8944 Å have been measured for the wavelength range from 0.5 to 30 Å from the line centers using a tungsten ribbon light source, cell lengths L from 0.31 to 6.1 cm, and Cs densities N from 2×10^{14} to 2×10^{16} cm^{-3}. The wavelength dependence of the absorption coefficients are consistent with a Lorentzian form and values of $\gamma f/N=1.08\times10^{-7}$ and 0.30×10^{-7} cm^3 sec^{-1} are obtained for 8521 and 8944 Å lines. Here γ is the collisional (or Lorentzian) half-width and f is the oscillator strength. The values of $\gamma f/N$ deduced from total fractional absorption data agree with those determined from the line profiles. Our results agree well (to within 15%) with those of Gregory and with theory, but disagree with more recent data. A source of error in some previous determinations of half-widths is the fact that even when the calculated absorption is very large, the measured transmission at the line center is significant; about 3.5×10^{-2} compared to $\sim10^{-100,000}$ predicted from our measurements in the wings of the lines for $N=1.14\times10^{15}$ cm^{-3} and $L=5.9$ cm. This effect is shown to result from transmission through the monochromator at wavelengths in the far wings of the instrument function.

I. INTRODUCTION

The broadening of cesium resonance lines, Cs 8521 Å ($6^2P_{3/2}-6^2S_{1/2}$) and Cs 8944 Å ($6^2P_{1/2}-6^2S_{1/2}$), due to collisions with Cs atoms has been studied by several investigators. However, there is a two-order-of-magnitude discrepancy between the collisional half-widths[1] given by the early work of Gregory[2] and the recent data of Pollock and Jensen[3] for the Cs 8521 Å resonance line. As pointed out by Reck, Takebe, and Mead,[4] a significant difference between the two studies is in the method of interpretation of the data. Gregory[2] deduced the collisional half-width for the cesium resonance lines from the wings of the absorption line profile, while Pollock and Jensen[3] obtained their value from the width at half maximum of the apparent absorption coefficient curve. This difference has led to the proposal[4] that theories of collision broadening applicable in wings of the line are not valid near the resonance line center. Our objectives are to measure carefully the absorption coefficients in the same spectral range as in the earlier experiments and to determine accurate values for the self-broadening collision frequencies for the lowest resonance states of cesium. In the course of this work we have found one possible cause of the disparity among the frequencies for self-broadening collisions obtained in previous experiments. The experimental apparatus and procedures are reported in Sec. II. A theoretical treatment of the experiment is presented in Sec. III, and the results are given in Sec. IV. Section V contains a discussion of the present work and its relation to earlier work.

II. EXPERIMENTAL APPARATUS AND PROCEDURES

A schematic diagram of the experimental arrangement is shown in Fig. 1. It consists of a light source, an absorption cell, and a photoelectric detection system. The light source is a 100-100-W tungsten-strip projection lamp (Westinghouse EDW), which is housed in a blackened aluminum box and is powered by a current-regulated (0.01%), dc power supply. The lamp has brightness temperature of 2490°K as measured by a calibrated Leeds and Northrup optical pyrometer. Light emitted from this lamp is collimated by an

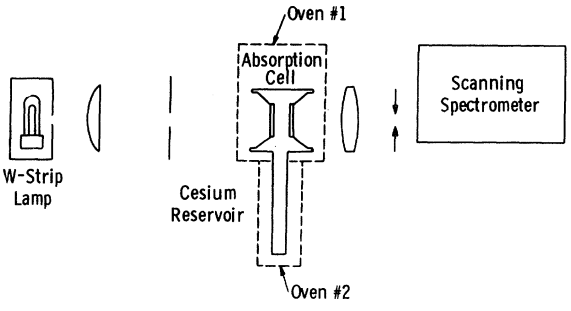

FIG. 1. Schematic diagram of the experimental setup.