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NOTE

NOTE ON THE INTERNAL CONSISTENCY OF THE SIGNS IN THE MATRIX OF $S^{1/2}$

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Abstract—A discrepancy in the evaluation of the sign of the quantity $S^{1/2}$ is stated. The SHORE and MENZEL[1] phases differ from the CONDON and SHORTLEY[2] phases for transitions from J to $J+1$. This result is a consequence of the fact that the first pair of authors consider $S^{1/2}$ as transforming like a reduced matrix element, while the second take $S^{1/2}(\alpha J, \alpha' J')$ as transforming like the quantity $(\alpha J \vdots P \vdots \alpha' J')$. The discrepancy in signs is removed if one looks at the relation between the reduced matrix element and the matrix element and the quantity $(\alpha J \vdots P \vdots \alpha' J')$. The CONDON and SHORTLEY[2] determination of the phase is more trustworthy, since for every breakdown of the LS-coupling from αJ to ΓJ the value of the line strength of the inverse transition equals the value of the line strength of the transition involved, which is not necessarily the case with the Shore and Menzel treatment. It is pointed out that in the case that the quantum numbers J do not get mixed up, it does not matter by which method the sign of $S^{1/2}$ is determined.

THE QUANTITY $S(\alpha J, \alpha' J')$ is called the line strength of the transition from the level αJ to the level $\alpha' J'$. This line strength is defined as the sum $\Sigma_{MM'}|\langle \alpha JM|P|\alpha' J'M'\rangle|^2$ of the absolute squares of the components of the electric dipole moment (SHORTLEY[3]).

According to GÜTTINGER and PAULI[4] (equation (23)), this line strength $S(\alpha J, \alpha' J')$ can be expressed as a function of quantities $(\alpha J \vdots P \vdots \alpha' J')$ with the aid of the following formula:

$$S(\alpha J, \alpha' J') = (2J+1)|(\alpha J \vdots P \vdots \alpha' J')|^2 \Xi(J, J') \tag{1}$$

with

$$\Xi(J, J+1) = (J+1)(2J+3)$$
$$\Xi(J, J) = J(J+1)$$
$$\Xi(J, J-1) = J(2J-1)$$

The quantity $S^{1/2}(\alpha J, \alpha' J')$ is defined as the square root of the line strength $S(\alpha J, \alpha' J')$ taken with the sign of $(\alpha J \vdots P \vdots \alpha' J')$ (SHORTLEY,[3] CONDON and SHORTLEY[2]).

The energy matrix of a certain configuration in an arbitrary coupling scheme is given, in general, by a Hermitian matrix $\langle \Gamma_i J_i|H|\Gamma_j J_j\rangle$, where $\Gamma_i J_i$ is the set of quantum numbers which defines the i-th energy level of the configuration involved. This Hermitian matrix can always be diagonalized by a unitary transformation, the diagonal matrix then being given by the matrix relation

$$\langle \alpha_k J_k|H|\alpha_l J_l\rangle = \langle \alpha_k J_k|\Gamma_i J_i\rangle\langle \Gamma_i J_i|H|\Gamma_j J_j\rangle\langle \Gamma_j J_j|\alpha_l J_l\rangle \tag{2}$$

where $\langle\alpha_k J_k|\Gamma_i J_i\rangle$ and $\langle\Gamma_j J_j|\alpha_l J_l\rangle$ are mutually inverse unitary matrices, uniquely defined by the unitary transformation.

The value of $S(\Gamma J, \Gamma' J')$ in the new coupling scheme is obtained by taking the square of the value of $S^{1/2}(\Gamma J, \Gamma' J')$ which can be found in its turn by multiplying the matrix containing $S^{1/2}(\alpha J, \alpha' J')$ as elements with the unitary matrices arising from the diagonalization of $\langle\alpha_k J_k|H|\alpha_l J_l\rangle$ and $\langle\alpha'_k J'_k|H|\alpha'_l J'_l\rangle$ respectively, as in equation (2), so that

$$S^{1/2}(\Gamma J, \Gamma' J') = \langle\Gamma J|\alpha J\rangle S^{1/2}(\alpha J, \alpha' J')\langle\alpha' J'|\Gamma' J'\rangle \tag{3}$$

holds as a matrix equation.

This result clearly shows the importance of determining the signs of the quantities $S^{1/2}(\alpha J, \alpha' J')$, which can be done by the method of CONDON and SHORTLEY[2] (p. 277). One can easily see that, in this case,

$$S^{1/2}(\alpha J, \alpha' J') = S^{1/2}(\alpha' J', \alpha J). \tag{4}$$

From the fact that the Hermitian matrix is also real (and thus symmetric), it follows that for the unitary matrices $\langle\Gamma J|\alpha J\rangle$ the inverse matrix $\langle\Gamma J|\alpha J\rangle^{-1}$ equals the transposed matrix $\langle\Gamma J|\alpha J\rangle$. Thus

$$\langle\Gamma J|\alpha J\rangle^{-1} = {}^{t}\langle\Gamma J|\alpha J\rangle = \langle\alpha J|\Gamma J\rangle \tag{5}$$

From equations (4) and (5) one easily finds the following important relation

$$S(\Gamma J, \Gamma' J') = S(\Gamma' J', \Gamma J) \tag{6}$$

The signs (or phases) obtained with the aid of the tables of SHORE and MENZEL[1] differ from the CONDON and SHORTLEY[2] phases by a factor (-1) in the case that $J' = J+1$, as appears clearly in the tables in several examples. In this case, one easily finds that

$$S^{1/2}(\alpha J, \alpha' J') = (-1)^{J-J'} S^{1/2}(\alpha' J', \alpha J) \tag{7}$$

so that equation (6) should not hold generally.

On the other hand, one can easily see that equation (7) will not invalidate equation (6) if one takes the electrostatic interaction, the spin-orbit interaction, the spin-orbit, and the spin–spin interaction (these last two effects involve different electrons) into account. In this case, the energy matrix does not contain elements connecting states with different value of J, as has been pointed out by YAMANOUCHI and HORIE;[5] thus $\langle\Gamma_i J_i|H|\Gamma_j J_j\rangle = 0$, if $J_i \neq J_j$.

The discrepancy in signs is, in fact, not surprising, since Condon and Shortley take the quantities $(\alpha J \vdots P \vdots \alpha' J')$ as transforming like the components of a matrix of an observable, while Shore and Menzel use the reduced matrix element $(\alpha J\|\mathbb{P}\|\alpha' J')$.

This reduced matrix element is defined by the fact that the electric-dipole operator is an example of an irreducible tensor operator of order 1, and that for such a quantity the Wigner–Eckardt theorem holds, which is, following the notation of DE SHALIT and TALMI:[6]

$$\langle\alpha JM|e\mathbb{R}_{\varkappa}^{(1)}|\alpha' J'M'\rangle = (-1)^{J-M}\begin{pmatrix} J & 1 & J' \\ -M & \varkappa & M' \end{pmatrix}(\alpha J\|e\mathbb{R}^{(1)}\|\alpha' J') \tag{8}$$

Here $\mathbb{P} = e\mathrm{R}^{(1)}$ with $e\mathrm{R}^{(1)}_{\varkappa}$ ($\varkappa = -1, 0, +1$) as components;

$\begin{pmatrix} J1J' \\ -M\varkappa M' \end{pmatrix}$ is a Wigner-coefficient or $3-j$ symbol.

TABLE 1

p^2p \ p^2s	(^{1}S) $^2S_{1/2}$	(^{3}P) $^2P_{1/2}$	(^{3}P) $^4P_{1/2}$	(^{3}P) $^2P_{3/2}$	(^{3}P) $^4P_{3/2}$	(^{1}D) $^2D_{3/2}$	(^{3}P) $^4P_{5/2}$	(^{1}D) $^2D_{5/2}$
J = 1/2 (^{1}S) ^{2}P	⊕ ⊞							
J = 1/2 (^{3}P) ^{2}S		⊖ ⊟		⊖ ⊞				
J = 1/2 (^{3}P) ^{2}P		⊕ ⊞		⊖ ⊞				
J = 1/2 (^{3}P) ^{4}P			⊖ ⊟		⊖ ⊞			
J = 1/2 (^{3}P) ^{4}D			⊕ ⊞		⊖ ⊞			
J = 1/2 (^{1}D) ^{2}P						⊖ ⊞		
J = 3/2 (^{1}S) ^{2}P	⊕ ⊞							
J = 3/2 (^{3}P) ^{2}P		⊖ ⊟		⊕ ⊞				
J = 3/2 (^{3}P) ^{2}D		⊕ ⊞		⊕ ⊞				
J = 3/2 (^{3}P) ^{4}S			⊕ ⊞		⊖ ⊟		⊖ ⊞	
J = 3/2 (^{3}P) ^{4}P			⊖ ⊟		⊕ ⊞		⊖ ⊞	
J = 3/2 (^{3}P) ^{4}D			⊕ ⊞		⊕ ⊞		⊖ ⊞	
J = 3/2 (^{1}D) ^{2}P						⊖ ⊟		⊖ ⊞
J = 3/2 (^{1}D) ^{2}D						⊕ ⊞		⊖ ⊞
J = 5/2 (^{3}P) ^{2}D				⊕ ⊞				
J = 5/2 (^{3}P) ^{4}P					⊖ ⊟		⊕ ⊞	
J = 5/2 (^{3}P) ^{4}D					⊕ ⊞		⊕ ⊞	
J = 5/2 (^{1}D) ^{2}D						⊖ ⊟		⊕ ⊞
J = 5/2 (^{1}D) ^{2}F						⊕ ⊞		⊕ ⊞
J = 7/2 (^{3}P) ^{4}D							⊕ ⊞	
J = 7/2 (^{1}D) ^{2}F								⊕ ⊞

TABLE 2

pp

ps	$^1S_0$	$^3P_0$	$^1P_1$	$^3S_1$	$^3P_1$	$^3D_1$	$^1D_2$	$^3P_2$	$^3D_2$	$^3D_3$
$^3P_0$				⊕ ⊞	⊖ ⊟	⊕ ⊞				
$^1P_1$	⊖ ⊞		⊕ ⊟				⊕ ⊞			
$^3P_1$		⊖ ⊞		⊖ ⊞	⊕ ⊟	⊕ ⊟		⊖ ⊟	⊕ ⊞	
$^3P_2$				⊖ ⊞	⊖ ⊞	⊖ ⊞		⊕ ⊟	⊕ ⊟	⊕ ⊞

p^2

ps	$^1S_0$	$^3P_0$	$^3P_1$	$^1D_2$	$^3P_2$
$^3P_0$			⊖ ⊟		
$^1P_1$	⊖ ⊞			⊕ ⊞	
$^3P_1$		⊖ ⊞	⊕ ⊟		⊖ ⊟
$^3P_2$			⊖ ⊞		⊕ ⊟

The tables include the sign of $S^{1/2}$ for the transitions $ps \rightarrow pp$, $p^2p \rightarrow p^2s$ and $ps \rightarrow p^2$. The signs in a square stand for the Shore and Menzel phases, the encircled signs denote the CONDON and SHORTLEY[2] phases. The broad, broken line shows that internal consistency breaks down for transitions by which J changes into $J+1$. For the inverse transitions, the ensquared signs change like $(-1)^{J-J'}$, while the encircled signs remain constant, so that the internal consistency again breaks down for the transitions from J to $J+1$.

Since $e\mathbb{R}^{(1)}$ is a Hermitian tensor, the following equation holds for the real reduced matrix elements:

$$(\alpha J\|\mathbb{P}\|\alpha' J') = (-1)^{J-J'}(\alpha' J'\|\mathbb{P}\|\alpha J) \tag{9}$$

Hence, according to equation (7), in the SHORE and MENZEL[1] scheme, the quantities $S^{1/2}$ transform like and take the signs of the corresponding reduced matrix elements.

The quantities $(\alpha J\|\mathbb{P}\|\alpha' J')$ and $(\alpha J \vdots P \vdots \alpha' J)$ are, according to RACAH;[7] formula (30) related by

$$\begin{aligned}(\alpha J\|\mathbb{P}\|\alpha' J) &= [J(J+1)(2J+1)]^{1/2}(\alpha J \vdots P \vdots \alpha' J)\\ (\alpha J\|\mathbb{P}\|\alpha' J-1) &= [J(2J-1)(2J+1)]^{1/2}(\alpha J \vdots P \vdots \alpha' J-1)\\ (\alpha J\|\mathbb{P}\|\alpha' J+1) &= -[(J+1)(2J+1)(2J+3)]^{1/2}(\alpha J \vdots P \vdots \alpha' J+1).\end{aligned} \tag{10}$$

From these expressions, it follows that

$$S(\alpha J, \alpha' J') = (\alpha J \| e\mathbf{R}^{(1)} \| \alpha' J')^2. \tag{11}$$

Equation (11) is certainly a simpler relation than equation (1), but, since $S^{1/2}(\alpha J, \alpha' J')$ takes the sign of $(\alpha J \vdots P \vdots \alpha' J')$, one easily finds that

$$S^{1/2}(\alpha J, \alpha' J') = \pm(\alpha J \| e\mathbf{R}^{(1)} \| \alpha' J') \tag{12}$$

where the plus-sign holds for $J' \neq J+1$ (thus $J' = J-1$ or $J' = J$) and the minus-sign holds for the case that $J' = J+1$.

If one applies this procedure to the SHORE and MENZEL[1] tables, one sees that the disagreement with the CONDON and SHORTLEY[2] phases is removed. This result means that, for any transition, the signs are in both cases internally consistent, which is the stated requirement. It is proposed that for the cases for which only internal consistency of the signs of $S^{1/2}$ is required, one should use the Shore and Menzel signs for $J' = J-1$ and $J' = J$ and invert these signs for $J' = J+1$.

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