Wigner relationships connecting fully differential dipole matrix elements to reduced matrix elements

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Abstract

Tabulated dipole matrix elements of the form $\langle n'l'j'||x||nlj\rangle$ can often be found in the literature. However, very often transition matrices between m-resolved states must be used. Furthermore, transitions between hyperfine-split levels must often be known. Finally, transition matrices between hyperfine-resolved and -unresolved levels may be required. Here, we present such matrix elements in terms of the unresolved elements.

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I. INTRODUCTION

Suppose I want to do a computation that requires me to know dipole transition matrices. And suppose I need to know transition matrices between fine-structure-resolved (FSR) states. Or suppose I need to know transition matrices between hyperfine-structure-resolved (HFSR)transitions. Finally, suppose I need to know transition matrices between FSR and HFSR states. In principle, I could deduce all of these knowing just the reduced matrix elements $\langle \gamma' l' || x || \gamma l \rangle$. That is, given these reduced matrix elements I should be able to deduce the following:

$$\langle \gamma' l' m_l' | x_q | \gamma l m_l \rangle \text{ , for all possible } m_l \text{ and } m_l' \tag{1a}$$

$$\langle \gamma' l' j' | x | \gamma l j \rangle \text{ , given } s\text{, for all possible } j \text{ and } j' \tag{1b}$$

$$\left\langle \gamma' l' j' m_j' | x_q | \gamma l j m_j \right\rangle \text{ , given } s\text{, for all possible } m_j \text{ and } m_j' \tag{1c}$$

$$\langle \gamma' l' j' I F' | x | \gamma l j I F \rangle \text{ , for all possible } F \text{ and } F' \tag{1d}$$

$$\langle \gamma' l' j' I F' m_F' | x_q | \gamma l j I F' m_F' \rangle \text{ , for all possible } m_F \text{ and } m_F'. \tag{1e}$$

$$\langle \gamma' l' j' F m_F | x_q | \gamma l j m_j \rangle \text{ , for all possible } F,\ m_F, \text{ and } m_j. \tag{1f}$$

II. THE SOLUTION

From Edmonds[1], Eq. 5.4.1,

$$\langle \gamma' j' m' | T_k | \gamma j m \rangle = (-1)^{j'-m'} \begin{pmatrix} j' & k & j \\ -m' & q & m \end{pmatrix} \langle \gamma' j' || T || \gamma j \rangle \tag{2}$$

In Eq. 2, the matrix-like expression is the Wigner 3-J symbol and q takes on values of -1, 0, +1 which correspond, respectively, to left-circularly polarized, linearly polarized, and right circularly polarized light. The argument k refers to the order of the transition. That is, $k = 1$ refers to dipole radiation, $k = 2$ means quadrupole radiation, etc. In this document we limit ourselves to electric dipole radiation, the operator for which we represent by x. We can use Eq. 2 to directly compute the matrix elements in expressions 1a, 1c and 1e:

$$\langle \gamma' l' m_l' | x_q | \gamma l m_l \rangle = (-1)^{l'-m_l'} \begin{pmatrix} l' & 1 & l \\ -m_l' & q & m_l \end{pmatrix} \langle \gamma' l' || x || \gamma l \rangle \tag{3a}$$

$$\left\langle \gamma' l' j' m_j' | x_q | \gamma l j m_j \right\rangle = (-1)^{j'-m_j'} \begin{pmatrix} j' & 1 & j \\ -m_j' & q & m_j \end{pmatrix} \langle \gamma' l' j' || x || \gamma l j \rangle \tag{3b}$$

$$\langle \gamma' l' j' I F' m_F' | x_q | \gamma l j I F' m_F' \rangle = (-1)^{F'-m_F'} \begin{pmatrix} F' & 1 & F \\ -m_F' & q & m_F \end{pmatrix} \langle \gamma' l' j' I F' || x || \gamma l j I F \rangle \tag{3c}$$

Now from Edmonds[1], Eq. 7.1.8,

$$\langle \gamma' j_1 j_2' J' | T_k | \gamma j_1 j_2 J \rangle = (-1)^{j_1+j_2+J'+k} \sqrt{(2J+1)(2J'+1)} \begin{Bmatrix} j_2' & J' & j_1 \\ J & j_2 & k \end{Bmatrix} \langle \gamma' j_2' || T_k || \gamma j_2 \rangle , \tag{4}$$

where the expression in curly braces is the Wigner 6-J symbol. We can use Eq. 4 to help us with expressions 1b and 1d:

$$\langle \gamma' s l' j' | x_q | \gamma s l j \rangle = (-1)^{s+l+j'+1} \sqrt{(2j+1)(2j'+1)} \begin{Bmatrix} l' & j' & s \\ j & l & 1 \end{Bmatrix} \langle \gamma' l' || x || \gamma l \rangle , \tag{5a}$$

$$\langle \gamma' I j' F' | x_q | \gamma I j F \rangle = (-1)^{I+j+F'+1} \sqrt{(2F+1)(2F'+1)} \begin{Bmatrix} j' & F' & I \\ F & j & 1 \end{Bmatrix} \langle \gamma' j' || x || \gamma j \rangle . \tag{5b}$$

In the derivation of the matrix element in Eq. 1f, we follow O. L. Weaver[2] who uses Biedenharn's notation for vector coupling coefficients. These will be converted at the end to Wigner coefficients. Note that Weaver uses m for m_j.

A typical matrix element we need is

$$\langle nljFM_F | x_q \left(|n_1 l_1 j_1 m_1\rangle \, |IM_I\rangle \right) . \tag{6}$$

That is,

$$C \begin{matrix} j & I & F \\ m' & M_I' & M_F \end{matrix} \left(\langle nljm' | \, \langle IM_I' | \right) x_q \left(|n_1 l_1 j_1 m_1\rangle \, |IM_I\rangle \right) = \frac{\langle nlj || x || n_1 l_1 j_1 \rangle}{\sqrt{2j+1}} C \begin{matrix} j_1 & 1 & j \\ m_1 & q & m' \end{matrix} \delta_{M_I M_I'} C \begin{matrix} j & I & F \\ m' & M_I' & M_F \end{matrix} . \tag{7}$$

But there's a problem here: we need a matrix element from $|n_1 l_1 j_1 m_1\rangle$ in the unresolved hyperfine manifold to a particular state $nljFM_F\rangle$ in the hyperfine-resolved manifold. Therefore the matrix element has to somehow "know" which M_I it is coming from. Fortunately, the triangle rule bails us out: For the vector coupling coefficients to be non-zero, $m_1+q=m'$ and $m'+M_I=M_F$. Therefore our desired matrix element (6) is

$$\langle nljFM_F|x_q|n_1l_1j_1m_1\rangle = \frac{\langle nlj||x||n_1l_1j_1\rangle}{\sqrt{2j+1}} C\begin{matrix} j_1 & 1 & j \\ m_1 & q & m' \end{matrix} C\begin{matrix} j & I & F \\ m' & M_I & M_F \end{matrix}, \tag{8}$$

with

$$m' = m_1 + q \tag{9a}$$

$$M_I = M_F - m'. \tag{9b}$$

In terms of Wigner coefficients, and incorporating Eqs. 9, this becomes

$$\langle nljFM_F|x_q|n_1l_1j_1m_1\rangle = (-1)^{j_1-1+m_1+q+j-I+M_F}\, \langle nlj||x||n_1l_1j_1\rangle \sqrt{2F+1}\times$$
$$\begin{pmatrix} j_1 & 1 & j \\ m_1 & q & -(m_1+q) \end{pmatrix} \begin{pmatrix} j & I & F \\ m_1+q & M_F-(m_1+q) & -M_F \end{pmatrix}. \tag{10}$$

III. SUMMARY OF RESULTS

The original goal was to express all transition matrix elements in terms of $\langle \gamma' l'||x||\gamma l\rangle$. However, the actual transition rate also depends on the transition wavelength. Therefore if the fine-structure splitting is sufficiently large, for example for the alkali D-lines, it is possible that using $\langle \gamma' l'||x||\gamma l\rangle$ to obtain $\langle \gamma' l' j'||x||\gamma l j\rangle$ may not be sufficiently accurate. Therefore, we assume that reduced matrix elements of the form $\langle \gamma' l' j'||x||\gamma l j\rangle$ are available and we need only tabulate matrix elements in terms of this reduced matrix element. By combining the above results, these are summarized as:

$$\left\langle n'l'j'm_j'|x_q|nljm_j\right\rangle = (-1)^{j'-m_j'} \begin{pmatrix} j' & 1 & j \\ -m_j' & q & m_j \end{pmatrix} \langle n'l'j'||x||nlj\rangle \tag{11}$$

$$\begin{aligned} \langle n'l'j'IF'|x|nljIF\rangle = (-1)^{I+j+F'+1}\sqrt{(2F+1)(2F'+1)}\times \\ \begin{Bmatrix} j' & F' & I \\ F & j & 1 \end{Bmatrix} \langle n'l'j'||x||nlj\rangle \end{aligned} \tag{12}$$

$$\begin{aligned} \langle n'l'j'IF'm_F'|x_q|nljIFm_F\rangle = (-1)^{I+j+1+2F'-m_F'}\times \\ \sqrt{(2F+1)(2F'+1)} \begin{pmatrix} F' & 1 & F \\ -m_F' & q & m_F \end{pmatrix} \langle n'l'j'||x||nlj\rangle \end{aligned} \tag{13}$$

$$\begin{aligned} \langle n'l'j'IF'm_F'|x_q|nljm_jI\rangle = (-1)^{j+m_j-1+q+j'-I+m_F'}\sqrt{2F'+1}\times \\ \begin{pmatrix} j & 1 & j' \\ m_j & q & -(m_j+q) \end{pmatrix} \begin{pmatrix} j' & I & F' \\ m_j+q & m_F'-(m_j+q) & -m_F' \end{pmatrix} \langle n'l'j'||x||nlj\rangle \end{aligned} \tag{14}$$

$$\langle n'l'j'IF'|x_q|nljI\rangle = ???? \times \langle n'l'j'||x||nlj\rangle \tag{15}$$

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[1] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1960).

[2] O. L. Weaver, personal communication.