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Generalized Racah Coefficient and its Applications

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Generalized Racah coefficient, designated as U coefficient in this paper, has been defined as the transformation function between two different coupling schemes in pairs of any four angular momenta, corresponding to the Racah coefficient defined as the transformation function between two different coupling schemes of any three angular momenta. Several simple properties of the U coefficient have been derived, and the method of tensor operators made to be extended to more general problems. Transformation coefficients between LS- and jj-coupling schemes in a many particle system can be evaluated by making use of these coefficients.

§ 1. Introduction

The Racah coefficient has proved to play a very important role in detailed theories of the atomic and nuclear spectroscopy[1-3], and also to be useful for the studies of the nuclear radiations and reactions.[4),5)] It is defined as the transformation function between two different coupling schemes of any three angular momenta j_1, j_2 and j_3 by

$$[(2J_{12}+1)(2J_{23}+1)]^{1/2}W(j_1j_2\,Jj_3\,;\,J_{12}\,J_{23})=(j_1j_2(J_{12})j_3J\,|\,j_1,j_2j_3(J_{23})J),\quad (1)$$

where $\boldsymbol{j}_1+\boldsymbol{j}_2=\boldsymbol{J}_{12}$, $\boldsymbol{j}_2+\boldsymbol{j}_3=\boldsymbol{J}_{23}$ and $\boldsymbol{J}_{12}+\boldsymbol{j}_3=\boldsymbol{J}_1+\boldsymbol{J}_{23}=\boldsymbol{J}$. In a similar way, we can define the generalized Racah coefficient which is designated as the U coefficient in this paper, as the transformation function between two different coupling orders in pairs of any four angular momenta j_1, j_2, j_3 and j_4 by

$$[(2J_{12}+1)(2J_{34}+1)(2J_{13}+1)(2J_{24}+1)]^{1/2}U\begin{pmatrix} j_1 & j_2 & J_{12} \\ j_3 & j_4 & J_{34} \\ J_{13} & J_{24} & J \end{pmatrix}$$

$$=(j_1j_2(J_{12})j_3j_4(J_{34})J\,|\,j_1j_3(J_{13})j_2j_4(J_{24})J),\qquad (2)$$

where $\boldsymbol{j}_1+\boldsymbol{j}_2=\boldsymbol{J}_{12}, \boldsymbol{j}_3+\boldsymbol{j}_4=\boldsymbol{J}_{34}, \boldsymbol{j}_2+\boldsymbol{j}_4=\boldsymbol{J}_{24}$, $\boldsymbol{j}_1+\boldsymbol{j}_3=\boldsymbol{J}_{13}$ and $\boldsymbol{J}_{12}+\boldsymbol{J}_{34}=\boldsymbol{J}_{13}+\boldsymbol{J}_{24}=\boldsymbol{J}$, and the nine angular monenta as the arguments in the U coefficients are arranged in three rows and columns in natural order. It is, therefore, expressed by a sum of the products of six Clebsch-Gordan coefficients of the vector additions as

$$(j_1j_2(J_{12})j_3j_4(J_{34})J\,|\,j_1j_3(J_{13})j_2j_4(J_{24})J)=\sum(j_1j_2\,m_1m_2\,|\,j_1j_2J_{12}M)$$

$$\cdot(j_3j_4\,m_3m_4\,|\,j_3j_4J_{34}\,M_{34})\,(J_{12}J_{34}\,M_{12}\,M_{34}\,|\,J_{12}J_{34}\,JM)\,(j_1j_3\,m_1m_3\,|\,j_1j_3J_{13}M_{13})$$

$$\cdot(j_2j_4\,m_2\,m_4\,|\,j_2j_4\,J_{24}\,M_{24})\,(J_{13}J_{24}\,M_{13}\,M_{24}\,|\,J_{13}\,J_{24}JM),\qquad (3)$$

where the summation is extended over all possible values of $m_1, m_2, m_3, m_4, M_{12}, M_{34}, M_{13}$ and M_{24}, restricted by obvious relations $m_1+m_2=M_{12}$, $m_3+m_4=M_{34}$, $m_1+m_3=M_{13}$, $m_2+m_4=M_{24}$, and $M_{12}+M_{34}=M_{13}+M_{24}=M$.

It is shown in the next section, that the U coefficient can be expressed in terms of a sum of the products of three Racah coefficients and that the Racah coefficient is a special case of the U coefficient. Some other properties of the coefficient, also, will be derived there. In sec. 3, the method of tensor operators are extended to more general operators which are constructed as tensor products of two tensor operators. It enables us to treat the spin-dependent interactions in a more general way. And in sec. 4, the method of the calculation of the transformation function between LS- and jj-coupling schemes is derived which seems very important in the treatment of nuclear shell model, especially for light nuclei. Finally some recurrence formulae for the coefficients are given in the Appendix.

§ 2. Properties of the U coefficients

The U coefficient in (2) is defined for integral and half-integral values of the nine parameters, with the limitation that each of the six triads

$$(j_1, j_2, J_{12}),\ (j_3, j_4, J_{34}),\ (J_{12}, J_{34}, J),\ (j_1, j_3, J_{13}),\ (j_2, j_4, J_{24}),\ (J_{13}, J_{24}, J) \tag{4}$$

has an integral sum, and vanishes unless the elements of each triad (4) satisfy the triangular inequalities according to the definition (2) and (3).

The summation in (3) can be carried out by making use of the Racah coefficients if we introduce the following intermediate state characterised by $\boldsymbol{J}_{123}=\boldsymbol{J}_{12}+\boldsymbol{j}_3$, that is

$$\begin{aligned}&(j_1j_2(J_{12})j_3j_4(J_{34})J\,|\,j_1j_3(J_{13})j_2j_4(J_{24})J)\\ &=\sum_{J_{123}}(J_{12}, j_3j_4(J_{34})J\,|\,J_{12}j_3(J_{123})j_4J)\,(j_1j_2(J_{12})j_3J_{123}\,|\,j_1j_3(J_{13})j_2J_{123})\\ &\quad\cdot(J_{13}j_2(J_{123})j_4J\,|\,J_{13}, j_2j_4(J_{24})J),\end{aligned} \tag{5}$$

where the summation over J_{123} is extended over all possible values compatible with the condition $\boldsymbol{J}_{123}=\boldsymbol{J}_{12}+\boldsymbol{j}_3=\boldsymbol{J}_{13}+\boldsymbol{j}_2$. Therefore the U coefficient can be expressed in terms of Racah coefficients with RIII (4) and (5). In abbreviated notations for arguments, it is given by

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix}=\sum_\lambda(2\lambda+1)\,W(fgbd;\,f'\lambda)\,W(egcd;\,e'\lambda)\,W(fcbe;\,a\lambda). \tag{6}$$

It is easily seen that the Racah coefficient can be obtained as a special case of the U coefficient in which any one of the six arguments b, c, d, e, f and g appearing in any two W's in the right hand side is equal to zero. For example, if $g=0$, $e=e'$ and $f=f'$ result for non-vanishing U, which is given by

$$U\begin{pmatrix} a & b & e \\ c & d & e \\ f & f & 0 \end{pmatrix} = (-1)^{e+f-a-d}\, W(abcd;\, ef)/[(2e+1)(2f+1)]^{1/2}. \tag{7}$$

Owing to the symmetry properties of the U coefficient which we can show in the following, the coefficient reduces always to the W coefficient if any one of its nine arguments is equal to zero.

We can immediately derive the following symmetry properties from those of the Racah coefficients (see RII (40a) and (40b)) and the relations given by RII (43) and Biedenharn, Blatt and Rose's[6] (17).

i) Transposition of "rows" and "columns":

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix} = U\begin{pmatrix} a & c & f \\ b & d & f' \\ e & e' & g \end{pmatrix}. \tag{8}$$

ii) Interchanges of two "rows" or "columns";

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix} = (-1)^{\sigma} U\begin{pmatrix} c & d & e' \\ a & b & e \\ f & f' & g \end{pmatrix} = (-1)^{\sigma} U\begin{pmatrix} f & f' & g \\ c & d & e' \\ a & b & e \end{pmatrix}, \tag{9}$$

where $\sigma = a+b+c+d+e+e'+f+f'+g$ (=integer).

Combining (8) and (9), we obtain 72 different arrangements of the nine parameters. For example, we can rewrite formula (6) into the following more symmetrical form:

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix} = (-1)^{\sigma} \sum_{\lambda} (2\lambda+1)\, W(bcf;\, \lambda a)\, W(bcf'e';\, \lambda d)\, W(efe'f';\, \lambda g), \tag{10}$$

where the "diagonal" elements of U appear as the last arguments of the three W coefficients. We shall prefer this form as the standard formula connecting the U and the W coefficients. Furthermore, it is easy to see that, if $a=c$, $b=d$ and $e=e'$, according to (9),

$$U\begin{pmatrix} a & b & e \\ a & b & e \\ f & f' & g \end{pmatrix} = 0, \qquad (f+f'+g=\text{odd}). \tag{11}$$

Some identities can be derived from the definition of the U coefficient as a transformation function between two different couplings in pairs of four angular momenta. Four angular momenta a, b, c and d can be combined into various pairs, as follows:

$$\boldsymbol{g} = (\boldsymbol{a}+\boldsymbol{b}) + (\boldsymbol{c}+\boldsymbol{d}) = (\boldsymbol{a}+\boldsymbol{c}) + (\boldsymbol{b}+\boldsymbol{d}) = (\boldsymbol{a}+\boldsymbol{d}) + (\boldsymbol{b}+\boldsymbol{c}). \tag{12}$$

It follows at once that

$$\sum_{ff'}(ab(e)cd(e')g \mid ac(f)bd(f')g)(ac(f)bd(f')g \mid ab(e_1)cd(e_1')g)$$
$$=\delta(e, e_1)\delta(e', e_1'). \tag{13}$$

In terms of U's, this gives us from (2), the following orthogonality relation between them:

$$\sum_{ff'}(2f+1)(2f'+1)U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix}U\begin{pmatrix} a & b & e_1 \\ c & d & e_1' \\ f & f' & g \end{pmatrix}$$
$$=\delta(c, e_1)\delta(c', e_1')/[(2e+1)(2e'+1)]. \tag{14}$$

Since the transformation function between the first and third coupling orders in pairs of (12) can be expressed, through the second one, as

$$\sum_{ff'}(ab(e)cd(e')g \mid ac(f)bd(f')g)(ac(f)bd(f')g \mid ad(h)bc(h')g)$$
$$=(ab(e)cd(e')g \mid ad(h)bc(h')g), \tag{15}$$

we obtain, another useful relation between U's:*

$$\sum_{ff'}(-1)^{e'-f'-2c+h'}(2f+1)(2f'+1)U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix}U\begin{pmatrix} a & c & f \\ d & b & f' \\ h & h' & g \end{pmatrix}=U\begin{pmatrix} a & b & e \\ d & c & e' \\ h & h' & g \end{pmatrix}. \tag{16}$$

We can see without difficulties that (15) and (16) are the generalization of RII (42) and (43), if we put g equal to zero. Beside these relations we have obtained several other relations between U's and between U's and W's, some of which will be given in Appendix. We shall also show there how recurrence formulae for U coefficients are obtained from one of them.

§ 3. Application to the calculation of matrix elements of tensor operators

(a) Tensor product of two tensor operators

The tensor product of two tensor operators $\boldsymbol{T}^{(k_1)}$ and $\boldsymbol{U}^{(k_2)}$ is defined in the usual way by an irreducible form

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*) The following relations are easily proved:

$$(ab(c)cd(e')g|ad(f)bc(f')g)=(-1)^{c+d-e'}[(2e+1)(2e'+1)(2f+1)(2f'+1)]^{1/2}U\begin{pmatrix} a & b & e \\ d & c & e' \\ f & f' & g \end{pmatrix},$$

and

$$(ab(e)cd(e')g|ad(f)cb(f')g)=(-1)^{d-e'-b+f'}[(2e+1)(2e'+1)(2f+1)(2f'+1)]^{1/2}U\begin{pmatrix} a & b & e \\ d & c & e' \\ f & f' & g \end{pmatrix}.$$

$$[\boldsymbol{T}^{(k_1)}\times\boldsymbol{U}^{(k_2)}]_Q^{(K)}=\sum_{q_1q_2}T_{q_1}^{(k_1)}\cdot U_{q_2}^{(k_2)}(k_1k_2q_1q_2\mid k_1k_2KQ). \tag{17}$$

In practical applications the most important tensor products are those in which two tensor operators operate on different parts of a composite system. The operator of this type appears in many problems, for example, in the calculation of matrices of spin-dependent interactions[7-9], of multipole moments of radiations in the nuclear shell model[10], and of polarization of emerging particles in nuclear reactions[11].*

When $\boldsymbol{T}^{(k_1)}$ operates on system 1 and $\boldsymbol{U}^{(k_2)}$ operates on system 2, the matrix element of a tensor product of $\boldsymbol{T}^{(k_1)}$ and $\boldsymbol{U}^{(k_2)}$ in (j_1j_2JM) scheme is given by

$$\begin{aligned}(j_1j_2JM\mid[\boldsymbol{T}^{(k_1)}\times\boldsymbol{U}^{(k_2)}]_Q^{(K)}\mid j_1'j_2'J'M')&=\sum(j_1j_2JM\mid j_1j_2m_1m_2)\\&\cdot(j_1m_1\mid T_{q_1}^{(k_1)}\mid j_1'm_1')(j_2m_2\mid U_{q_2}^{(k_2)}\mid j_2'm_2')\\&\cdot(j_1'j_2'm_1'm_2'\mid j_1'j_2'J'M')(k_1k_2q_1q_2\mid k_1k_2KQ).\end{aligned}\tag{18}$$

And, if the double-barred element is defined in accordance with RII (29) by

$$(\alpha jm\mid T_q^{(k)}\mid\alpha'j'm')=(\alpha j\parallel T^{(k)}\parallel\alpha'j')(j'km'q\mid j'kjm)/(2j+1)^{1/2}, \tag{19}$$

it is easy to be shown that the double-barred elements of the tensor product $[\boldsymbol{T}^{(k_1)}\times\boldsymbol{U}^{(k_2)}]^{(K)}$ are expressed in terms of those of $\boldsymbol{T}^{(k_1)}$ and $\boldsymbol{U}^{(k_2)}$ and a U coefficient as follows:

$$\begin{aligned}(j_1j_2J\parallel[T^{(k_1)}\times U^{(k_2)}]^{(K)}\parallel j_1'j_2'J')&=(j_1\parallel T^{(k_1)}\parallel j_1')(j_2\parallel U^{(k_2)}\parallel j_2')\\&\cdot[(2J+1)(2J'+1)(2K+1)]^{1/2}U\begin{pmatrix}j_1&j_1'&k_1\\j_2&j_2'&k_2\\J&J'&K\end{pmatrix}.\end{aligned}\tag{20}$$

This simple and symmetrical formula is a natural generalization of RII (38), (44a) and (44b). First of all, noting that

$$(\boldsymbol{T}^{(k)}\cdot\boldsymbol{U}^{(k)})=(-1)^k(2k+1)^{1/2}[T^{(k)}\times U^{(k)}]^{(0)}_0 \tag{21}$$

where in the left-hand side $(\boldsymbol{T}^{(k)}\cdot\boldsymbol{U}^{(k)})=\sum_q(-1)^qT_q^{(k)}U_{\bar{q}}^{(k)}$ represents the scalar product of the two tensor operators $\boldsymbol{T}^{(k)}$ and $\boldsymbol{U}^{(k)}$, and putting $k_1=k_2=k$ and $K=0$ in (20), we obtain the relation RII (38)

$$\begin{aligned}(j_1j_2JM\mid(\boldsymbol{T}^{(k)}\cdot\boldsymbol{U}^{(k)})\mid j_1'j_2'JM)&=(-1)^{j_1+j_2'-J}\\&\cdot(j_1\parallel T^{(k)}\parallel j_1')(j_2\parallel U^{(k)}\parallel j_2')W(j_1j_2j_1'j_2';Jk).\end{aligned}\tag{22}$$

Putting further $k_2=0$ and $k_1=K=k$ in (20), and noting that $(j\parallel 1\parallel j)=(2j+1)^{1/2}$, we get the relation given by RII (44a)

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*) For the same coefficient as our U's, U. Fano and G. Racah seem to have given the notation $X(abe;cde';ff'g)$ in their unpublished paper (cf. ref. 11).

$$(j_1 j_2 J \| T^{(k)} \| j_1' j_2 J') = (-1)^{k+j_2-j_1'-J}$$
$$\cdot (j_1 \| T^{(k)} \| j_1') [(2J+1)(2J'+1)]^{1/2} W(j_1 J j_1' J' ; j_2 k). \tag{23}$$

The relation RII (44b) can be obtained in a similar way by putting $k_1=0$ and $k_2=K=k$.

It must be observed that for the double-barred elements of the tensor product,

$$(j_1 j_2 J \| [T^{(k_1)} \times U^{(k_2)}]^{(K)} \| j_1' j_2' J') = (-1)^{J-J'+k_1+k_2-K}$$
$$\cdot (j_1' j_2' J' \| [T^{(k_1)} \times U^{(k_2)}]^{(K)} \| j_1 j_2 J), \tag{24}$$

corresponding to RII (31). As a special case of (24), the following formula is obtained, by putting $j_1=j_1'$, $j_2=j_2'$ and $J=J'$,

$$(j_1 j_2 J \| [T^{(k_1)} \times U^{(k_2)}]^{(K)} \| j_1 j_2 J) = 0 \qquad (k_1+k_2-K=\text{odd}), \tag{25}$$

which can also be derived from (11) immediately.

(b) Matrix elements of the scalar product of two irreducible composite tensors

In order to calculate the matrix of spin-dependent interactions, it is necesary to treat the scalar product of two irreducible composite tensors. Hence we consider this quantity more in detail. Let $\boldsymbol{T}^{(k_1 k_2 ; K)}$ be an irreducible composite tensor of degree K with respect to $\boldsymbol{J}=\boldsymbol{j}_1+\boldsymbol{j}_2$ which behaves as an irreducible tensor of degree k_1 and k_2 with respect to j_1 and j_2 respectively (This may be considered as an abbreviation of the tensor product given in (17)), and $\boldsymbol{U}^{(k_1 k_2 ; K)}$ have a similar meaning. By making use of (20) and BBR (1), the matrix elements of this scalar product in $(j_1 j_2 JM)$ scheme are given by

$$(\gamma j_1 j_2 JM | (\boldsymbol{T}^{(k_1 k_2 ; K)} \cdot \boldsymbol{U}^{(k_1 k_2 ; K)}) | \gamma j_1' j_2' JM)$$
$$= (2K+1) \sum_{\gamma'' j_1'' j_2''} (\gamma j_1 j_2 \| T^{(k_1, k_2)} \| \gamma'' j_1'' j_2'') (\gamma'' j_1'' j_2'' \| U^{(k_1, k_2)} \| \gamma' j_1' j_2')$$
$$\cdot \sum_{J''} (-1)^{J-J''} (2J''+1)\, U\begin{pmatrix} j_1 & j_1'' & k_1 \\ j_2 & j_2'' & k_2 \\ J & J'' & K \end{pmatrix} U\begin{pmatrix} j_1'' & j_1' & k_1' \\ j_2'' & j_2' & k_2' \\ J'' & J & K \end{pmatrix}. \tag{26}$$

The summation over J'' in (26) can be carried out, using the relation between U and W coefficients and with RII (43) and BBR (17), so that (26) is written in an expected form as

$$(\gamma j_1 j_2 JM | (T^{(k_1 k_2 ; K)} \cdot U^{(k_1' k_2' ; K)}) | \gamma' j_1' j_2' JM)$$
$$= (2K+1) \sum_{\lambda} (-1)^{j_1+j_2'-J} W(j_1 j_2 j_1' j_2' ; J\lambda)$$
$$\cdot \sum_{\gamma'' j_1'' j_2''} (-1)^{k_1'+k_2} (\gamma j_1 j_2 \| T^{(k_1, k_2)} \| \gamma'' j_1'' j_2'') (\gamma'' j_1'' j_2'' \| U^{(k_1', k_2')} \| \gamma' j_1' j_2')$$
$$\cdot W(j_1 j_2' k_1 k_2' ; \lambda j_1'') W(j_2 j_2' k_2 k_3' ; \lambda j_2'') W(k_1 k_2 k_1' k_2' ; K\lambda). \tag{27}$$

This formula is useful, especially, in the treatment of the spin-dependent interactions[7-9], in which this reduction has been done in a more straightforward way. For example, in the case of the spin-spin interaction between electrons, the angular momenta j_1 and j_2 are the total spin and the total orbital angular momenta respectively, and $k_1=k_1'=1$ and $k_2'=k_2+2$ ($k=0,\ 2,\cdots$), so that only $\lambda=2$ appears in this equation.

(c) Coefficients of the exchange integrals of a many particle system

Racah has given a general method for obtaining the coefficient of exchange integrals in the case of electrostatic interactions RII, sec. 5. We shall extend this method to spin-dependent interactions, making use of the result in this section. The spin-dependent interaction can be represented as a scalar product of two irreducible tensors which have degree K ($K\neq 0$) in the spin and the ordinary space respectively; for example, in the tensor or the spin-spin interaction $K=2$ and in the spin-orbit interaction $K=1$.

First, we consider only the orbital part and assume that the irreducible tensor is a tensor product of two tensor operators of degree k_1 and k_2, the former operating on particle 1 and the latter on particle 2. Then we obtain the orbital part of coefficients of exchange integrals in terms of double-barred elements as

$$(-1)^{l_1+l_2-L'}(l_1 l_2 L\,\|\,[T_1^{(k_1)}\times U_2^{(k_2)}]^{(K)}\,\|\,l_2 l_1 L')$$
$$=(-1)^{l_1+l_2-L'}(l_1\,\|\,T^{(k_1)}\,\|\,l_2)(l_2\,\|\,U^{(k_2)}\,\|\,l_1)[(2L+1)(2L'+1)(2K+1)]^{1/2}\cdot U\begin{pmatrix} l_1 & l_2 & L \\ l_1 & l_2 & L' \\ k_1 & k_2 & K \end{pmatrix},$$

and owing to (15) and RII (31), it follows that

$$(-1)^{l_1+l_2-L}(l_1 l_2 L\,\|\,[T^{(k_1)}\times U^{(k_2)}]^{(K)}\,\|\,l_2 l_1 L')$$
$$=(l_1\,\|\,T^{(k_1)}\,\|\,l_2)(l_1\,\|\,U^{(k_2)}\,\|\,l_2)[(2L+1)(2L'+1)(2K+1)]^{1/2}$$
$$\cdot\sum_{r,s}(-1)^{k_2-s}\cdot(2r+1)(2S+1)U\begin{pmatrix} l_1 & l_1 & r \\ l_2 & l_2 & s \\ k_1 & k_2 & K \end{pmatrix}U\begin{pmatrix} l_1 & l_2 & L \\ l_1 & l_2 & L' \\ r & s & K \end{pmatrix}. \tag{28}$$

Futhermore, if we define the unit tensor $u^{(k)}$ by

$$(l\,\|\,u^{(k)}\,\|\,l')=\delta(l,l'), \tag{29}$$

and take (20) into account, we may also write

$$(-1)^{l_1+l_2-L}(l_1 l_2 L\,\|\,[T^{(k_1)}\times U^{(k_2)}]^{(K)}\,\|\,l_2 l_1 L')$$
$$=(l_1\,\|\,T^{(k_1)}\,\|\,l_2)(l_1\,\|\,U^{(k_2)}\,\|\,l_2)\sum_{r,s}(-1)^{k_2-s}(2r+1)(2s+1)$$
$$\cdot U\begin{pmatrix} l_1 & l_1 & r \\ l_2 & l_2 & s \\ k_1 & k_2 & K \end{pmatrix}\cdot(l_1 l_2 L\,\|\,[u_1^{(r)}\times u_2^{(s)}]^{(K)}\,\|\,l_1 l_2 L'). \tag{30}$$

Therefore, the calculation of the coefficients of the exchange integrals can be carried out in the same way as for obtaining those of direct integrals with respect to the operator

$$(l_1 \| T^{(k_1)} \| l_2)(l_1 \| U^{(k_2)} \| l_2) \sum_{r,s} (-1)^{k_2-s}(2r+1)(2s+1)$$
$$\cdot U\begin{pmatrix} l_1 & l_1 & r \\ l_2 & l_2 & s \\ k_1 & k_2 & K \end{pmatrix} [\boldsymbol{u}_1^{(r)} \times \boldsymbol{u}_2^{(s)}]^{(K)}, \tag{31}$$

in place of $[\boldsymbol{T}^{(k_1)} \times \boldsymbol{U}^{(k_2)}]$. In a similar way, another irreducible tensor of degree K can be obtained as the spin part, which becomes usually much simpler. Therefore, the complete operator necessary for the calculation of coefficients of exchange integrals is given by contructing scalar products of these two irreducible tensors of degree K with respect to the ordinary and spin spaces and reversing the total sign due to the antisymmetry of the wave functions.

As a trivial example of this procedure, the formula RII (59) of the coefficient $g_k(l_1 l_2 L)$ for the electrostatic interaction is derived by putting $K=0$ and $T^{(k_1)} = U^{(k_2)} = C^{(k)}$ in (31) where $C_q^{(k)} = [4\pi/(2k+1)]^{1/2} \Theta(kq)\Phi(q)$. Another trivial example is given by the construction of Dirac's exchange operator with (30). Letting $l_1 = l_2 = 1/2$, $\boldsymbol{T}^{(0)} = \boldsymbol{U}^{(0)} = \boldsymbol{1}$, and noting that $\boldsymbol{1} = (2)^{1/2}\boldsymbol{u}^{(0)}$ and $\boldsymbol{s} = (3/2)^{1/2}\boldsymbol{u}^{(1)}$, we immediately have Dirac's exchange operator

$$(-1)^{1-S} = 1/2 \cdot [1 + 2(\boldsymbol{s}_2 \cdot \boldsymbol{s}_1)]. \tag{32}$$

The simplest example of the spin-dependent interactions is given by the spin-spin interaction between electrons.[7),8)] In this case, we need not change the form of the spin part since it is symmetrical with respect to the spin variables of two electrons. This holds also for the tensor interaction with arbitrary radial dependence. The coefficients of exchange integrals of the spin-spin interaction between electrons

$$\int\int R_{l_1}(r_1) R_{l_2}(r_2) \frac{r_1^{\,k}}{r_1^{\,k+3}} R_{l_1}(r_2) R_{l_2}(r_1)\, dr_1 dr_2$$

are given by the matrix elements of the operator

$$-2f_k(l_1 \| C^{(k)} \| l_2)(l_1 \| C^{k+2} \| l_2) \sum_{r,s}{}' (-1)^{k-s}(2r+1)(2s+1)$$
$$\cdot U\begin{pmatrix} l_1 & l_1 & r \\ l_2 & l_2 & s \\ k & k+2 & 2 \end{pmatrix} ([\boldsymbol{s}_1 \times \boldsymbol{s}_2]^{(2)} \cdot [\boldsymbol{u}_1^{(r)} \times \boldsymbol{u}_2^{(s)}]^{(2)}), \tag{33}$$

where the prime on the summation symbol denotes that the summation is extended only over those values of r and s which satisfy $r+s=$ even and the coefficients f_k is given by $(-1)^{k+1}4[(k+1)(k+2)(2k+1)(2k+3)(2k+5)/5]^{1/2}$.

§ 4. Transformation coefficients between *LS*- and *jj*-coupling schemes in l^n configuration

The transformation coefficient between LS- and jj-coupling schmes of two particle system can be obtained at once from the general expression for the transformation function between two different couplings in pairs of four angular momenta given in sec. 1 and 2. For two equivalent particles (identical particles which are contained in the same shell), however, the formula does not hold without modification on account of the Pauli exclusion principle as will be seen in the following. Here we consider the case in which there are n equivalent particles in the same shell with azimuthal quantum number l. The states of l^n configuration are characterized by $\alpha SLJM$ in LS-oupling scheme, where α is the quantum number other than S, L, J and M. On the other hand, the states with the same J and M are characterized by $j_1^{n_1}(\beta_1 J_1) j_2^{n_2}(\beta_2 J_2) JM$ in jj-coupling scheme, where $j_1 = l + 1/2$, $j_2 = l - 1/2$ and $n_1 + n_2 = n$, β's being the quantum number other than J and M. The quantum number of the isotopic spin employed sometimes in nuclear shell model can be included in α and in β. Taking into account the antisymmetry property of wave functions, the transformation function between LS- and jj-coupling schemes for n equivalent particles can be obtained in terms of those for $(n-1)$ equivalent particles, the coefficients of fractional parentages, and the U and W coefficients:

$$
\begin{aligned}
&(l^n\alpha SLJM\,|\,j_1^{n_1}(\beta_1 J_1) j_2^{n_2}(\beta_2 J_2) JM)\\
&=(-1)^{n_2}(n_1/n)^{1/2}\sum(l^n\alpha SL\{|\,l^{n-1}(\alpha' S'L')lsL)\Big(S'\tfrac{1}{2}(S)L'l(L)J\,|\,S'L'(J')\tfrac{1}{2}l(j_1)J\Big)\\
&\cdot(l^{n-1}\alpha' S'L'J'\,|\,j_1^{n_1-1}(\beta_1' J_1') j_2^{n_2}(\beta_2 J_2) J')(J_1' J_2(J') j_1 J\,|\,J_1' j_1(J_1) J_2 J)\\
&\cdot(j_1^{n_1-1}(\beta_1' J_1') j_1 J_1|\}\,j_1^{n_1}\beta_1 J_1)+(n_2/n)^{1/2}\sum(l^n\alpha SL\{|\,l^{n-1}(\alpha' S'L')lSL)\\
&\cdot\Big(S'\tfrac{1}{2}(S)L'l(L)J\,|\,S'L'(J')\tfrac{1}{2}l(j_2)J\Big)(l^{n-1}\alpha' S'L'J'\,|\,j_1^{n_1}(\beta_1 J_1) j_2^{n_2-1}(\beta_2' J_2') J')\\
&\cdot(J_1 J_2'(J') j_2 J\,|\,J_1, J_2' j_2(J_2) J)(j_2^{n_2-1}(\beta_2' J_2') j_2 J|\}\,j_2^{n_2}\beta_2 J_2).
\end{aligned}
\tag{34}
$$

The tables of the coefficients of fractional parentages were given by RIII for the atomic p^n and d^n configurations, by Jahn and van Wieringen[2] for the nuclear p^n, by Jahn[2] for d^3 and d^4 configurations in LS-coupling, and Edmond and Flowers[3] for $(3/2)^3$, $(3/2)^4$, $(5/2)^5$ $(7/2)^3$ and $(7/2)^4$ configurations. The tables of W coefficients were given by Biedenharn[12] and Obi *et al.*[13]

For two equivalent particles which have only states with $S+L=$ even in LS-coupling scheme, eq. (34) reduces to

$$
(l^2SLJM\,|\,j^2JM)=\Big(\tfrac{1}{2}\tfrac{1}{2}(S)ll(L)J\Big|\tfrac{1}{2}l(j)\tfrac{1}{2}l(j)J\Big),\qquad j=j_1 \text{ or } j_2,
$$

$$
(l^2SLJM\,|\,j_1 j_2 JM)=(2)^{1/2}\Big(\tfrac{1}{2}\tfrac{1}{2}(S)ll(L)J\Big|\tfrac{1}{2}l(j_1)\tfrac{1}{2}l(j_2)J\Big).
$$

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Appendix. Identities and recurrence formulae for the U coefficients

The values of the U coefficients can be obtained by inserting the values of the W coefficients in the formula (6). However, there are also some recurrence formulae between the U coefficients which may be available for the evaluation of the coefficients.

In order to obtain an identity from which recurrence formulae can be derived, we consider the following two different coupling schemes of five angular momenta and the transformation function between them. It is evident that

$$\begin{aligned}(j_1j_2(J_{12})j_3j_4(J_{34})(J_{1234})j_5J\,|\,j_1j_3(J_{13}),j_2j_4(J_{24})j_5(J_{245})J)\\ =(j_1j_2(J_{12})j_3j_4(J_{34})J_{1234}\,|\,j_1j_3(J_{13})j_2j_4(J_{24})J_{1234})\\ \cdot(J_{13}J_{24}(J_{1234})j_5J\,|\,J_{13},J_{24}j_5(J_{245})J).\end{aligned} \tag{A. 1}$$

But this transformation function can be expressed in another way by employing two intermediate state as

$$\begin{aligned}\sum_{J_{345}J_{45}}(J_{12}J_{34}(J_{1234})j_5J\,|\,J_{12},J_{34}j_5(J_{345})J)\,(j_3j_4(J_{34})j_5J_{345}\,|\,j_3,j_4j_5(J_{45})J_{345})\\ \cdot(j_1j_2(J_{12})j_3J_{45}(J_{345})J\,|\,j_1j_3(J_{13})j_2J_{45}(J_{245})J)\\ \cdot(j_2,j_4j_5(J_{45})J_{245}\,|\,j_2j_4(J_{24})j_5J_{245}).\end{aligned} \tag{A. 2}$$

Equating this with (A. 1) and expressing the result by the U and W coefficients, we obtain the relation between them as follows;

$$U\begin{pmatrix}a & b & e\\ c & d & e'\\ f & f' & g\end{pmatrix}W(ff'\bar{g}h;\,g\bar{f}')=\sum_{\lambda\mu}(2\lambda+1)(2\mu+1)\,W(ee'\bar{g}h;\,g\lambda)$$

$$\cdot W(cd\lambda h;\,e'\mu)\,W(bd\bar{f}'h;\,f'\mu)\,U\begin{pmatrix}a & b & e\\ c & \mu & \lambda\\ f & \bar{f}' & \bar{g}\end{pmatrix}. \tag{A. 3}$$

Applications of this identity to give recurrence formulae are immediate. Take, for example, $h=1/2$. Then in the summation on the right hand side of (A. 3) λ and μ take only two values $\lambda=e'\pm1/2$ and $\mu=d\pm1/2$ respectively. Then, we can choose the values of $\bar{f}'$ and $\bar{g}$ as $\bar{f}'=f'\pm1/2$ and $\bar{g}=g\pm1/2$. Therefore, the values of $U\begin{pmatrix}a & b & e\\ c & d-1/2 & e'-1/2\\ f & f'-1/2 & g-1/2\end{pmatrix}$, for example, can be evaluated in terms of four U coefficients

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix},\ U\begin{pmatrix} a & b & e \\ c & d & e'-1 \\ f & f' & g \end{pmatrix},\ U\begin{pmatrix} a & b & e \\ c & d-1 & e' \\ f & f' & g \end{pmatrix} \text{ and } U\begin{pmatrix} a & b & e \\ c & d-1 & e'-1 \\ f & f' & g \end{pmatrix}.$$

Coefficients of the relation which come from the W coefficients with one variable equal to 1/2, are simple algebraic functions. In a similar way, we can have a relation betwen the following nine U coefficients :

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix},\ U\begin{pmatrix} a & b & e \\ c & d & e'\pm1 \\ f' & f' & g \end{pmatrix},\ U\begin{pmatrix} a & b & e \\ c & d\pm1 & e' \\ f & f' & g \end{pmatrix} \text{ and } U\begin{pmatrix} a & b & e \\ c & d\pm1 & e'\pm1 \\ f & f' & g \end{pmatrix}.$$

Furthermore, it is easily shown that

$$(ab(e)c(e')dg \mid ad(f)c(f')eg)$$

$$=(-1)^{e-f-e'+f'}[(2e+1)(2e'+1)(2f+1)(2f'+1)]^{1/2}U\begin{pmatrix} a & e & b \\ f & c & f' \\ d & e' & g \end{pmatrix}. \qquad \text{(A.4)}$$

Using the definition (10) and (A, 4), we can find

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix}=(2g+1)\sum_{\lambda,\mu,\nu}(2\lambda+1)(2\mu+1)(2\nu+1)$$

$$\cdot U\begin{pmatrix} a & b & e \\ c & \bar{d} & \lambda \\ f & \mu & \nu \end{pmatrix} U\begin{pmatrix} \lambda & \nu & e \\ c & d & e' \\ \bar{d} & \bar{h} & g \end{pmatrix} U\begin{pmatrix} \mu & b & \bar{d} \\ \nu & d & \bar{h} \\ f & f' & g \end{pmatrix}, \qquad \text{(A. 5)}$$

and

$$U\begin{pmatrix} a & b & e \\ c & d & e' \\ f & f' & g \end{pmatrix} U\begin{pmatrix} \bar{a} & \bar{b} & \bar{e} \\ \bar{c} & \bar{d} & \bar{e}' \\ f & f' & g \end{pmatrix}=\sum_{\gamma_1,\gamma_2,\delta,\varepsilon}(-1)^{e'+\bar{a}-f'-\delta}(2\gamma_1+1)(2\gamma_2+1)(2\delta+1)(2\varepsilon+1)$$

$$\cdot U\begin{pmatrix} a & b & e \\ c & \varepsilon & \delta \\ f & \bar{a} & \bar{c} \end{pmatrix} U\begin{pmatrix} \bar{a} & \bar{b} & \bar{e} \\ \varepsilon & \bar{d} & \gamma_2 \\ b & f' & d \end{pmatrix} U\begin{pmatrix} c & d & e' \\ \varepsilon & \gamma_2 & \bar{d} \\ \delta & \bar{e} & \gamma_1 \end{pmatrix} U\begin{pmatrix} \bar{c} & \bar{d} & \bar{e}' \\ e & e' & g \\ \delta & \gamma_1 & \bar{e} \end{pmatrix}. \qquad \text{(A6)}$$

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