# Expansion of the spin-spin interaction

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The space part of a general spin-spin interaction is expanded in a complete orthonormal set of irreducible tensors constructed from spherical harmonics of the interacting particles. With this expansions, the $m$-scheme matrix element of the spin-spin interaction is represented as a sum of weighted radial integrals along with its graphical representation. The graphical form of the $m$-scheme matrix element enables one to obtain graphically matrix elements between many-particle configurations in any coupling scheme.

## I. INTRODUCTION

The progress in spectroscopic technology, e.g., electron spectroscopy for chemical analysis (ESCA), bent crystal, and optical interferometry with lasers, has provided an appreciable challenge to further atomic and molecular structure calculations including correlation and relativistic effects. To account for the correlation effects in many-particle systems (including atoms, molecules, and nuclei), correlated wave functions which explicitly contain interparticle distances $r_{ij}$ have been widely used. On the other hand, magnetic interactions in atoms, molecules, and nuclei are among the most interesting relativistic effects; a few recent formulations have been suggested.[1-3] The spin-spin interaction, in particular, has been expanded by many authors[3-10] in irreducible tensor form, which is appropriate only for states constructed from products of radial functions $\phi(r_i)$ and spherical harmonics $Y_{lm}(r_i)$. To evaluate the matrix element of the spin-spin interaction with correlated wave functions containing interparticle distances we have to consider, besides spherical harmonics accounting for the rotational symmetry of the states involved, a tensor operator of the general form

$$V_T=J(r_{12})[(\vec{\sigma}_1\cdot\vec{r}_{12})(\vec{\sigma}_2\cdot\vec{r}_{12})/r_{12}^2-\tfrac{1}{3}(\vec{\sigma}_1\cdot\vec{\sigma}_2)]\,. \quad (1)$$

Here $J(r_{12})$ is a scalar function possibly containing the correlated part of the wave functions, and $\vec{\sigma}_1$ and $\vec{\sigma}_2$ are the Pauli matrices of the respective particles. We note that the Fermi contact term[11] involving $\delta^3(\vec{r}_{12})$ in the spin-spin interaction can be evaluated trivially and is therefore not considered here. In a different context, the tensor operator (1) represents simply the general tensor force,[12] which is probably part of the actual nuclear interaction between nucleons and is required to describe nucleon-nucleon scatterings.

The tensor interaction (1) has been expanded by Talmi[13] in terms of irreducible tensors of each particle; however, the expansion is a complicated sum of tensor products and does not reflect its simple tensor properties. Nevertheless, the matrix element of (1) for harmonic oscillator functions can be evaluated by using the Moshinsky transformation brackets.[14] This alternative approach is, however, based on particular transformation relations between harmonic-oscillator functions and is not applicable for angular-momentum eigenfunctions in an arbitrary central field. The tensor interaction (1) can readily be written as a scalar product of two second-rank tensors involving spins and the vector $\vec{r}_{12}$, respectively. The tensor formed from the vector $\vec{r}_{12}$ has the form $f(r_{12})Y_{2m}(\hat{r}_{12})$, and it is this space part which needs attention. By a differential-equation method, Sack[15] has considered a more general function $f(r_{12})Y_{lm}(\hat{r}_{12})$ and obtained an expansion in operational form involving powers of differential operators, which is not in a convenient form for computational purposes.

In this work we shall expand the space part of (1) in a complete orthonormal set of irreducible tensors constructed from spherical harmonics of the two interacting particles. The $m$-scheme matrix element of the tensor interaction is also given in terms of radial integrals along with its graphical form. This graphical form of the $m$-scheme matrix element enables one to obtain matrix elements between many-particle configurations in any coupling scheme by adopting a graphical method.[16]

## II. IRREDUCIBLE TENSOR EXPANSION

It is well known that the tensor interaction (1) can be cast in a tensor product form

$$V_T=V(r_{12})[(\vec{r}_{12}\vec{r}_{12})_{2q}(\vec{\sigma}_1\vec{\sigma}_2)_{2p}]_{00}\,, \quad (2)$$

where the scalar function $V(r_{12})$ is

$$V(r_{12})=\sqrt{5}J(r_{12})/r_{12}^2\,. \quad (3)$$

The scalar product of two tensors is defined as

$$[(\vec{r}_{12}\vec{r}_{12})_{2q}(\vec{\sigma}_1\vec{\sigma}_2)_{2p}]_{00}=\sum_{qp}\langle 2q2p\,|00\rangle(\vec{r}_{12}\vec{r}_{12})_{2q}(\vec{\sigma}_1\vec{\sigma}_2)_{2p}\,, \tag{4}$$

where $\langle 2q2p\,|00\rangle$ is the Clebsch-Gordan coefficient.[17] Here $(\vec{\sigma}_1\vec{\sigma}_2)_{2p}$ is the irreducible tensor of rank 2 formed from $\vec{\sigma}_1$ and $\vec{\sigma}_2$, and $(\vec{r}_{12}\vec{r}_{12})_{2q}$ is that formed from the vector $\vec{r}_{12}$. By defining the Hermitian conjugate of a tensor operator $T_{jm}$ as

$$T^{\dagger}_{jm}=(-)^{j-m}T_{j-m}\,,$$

we can rewrite (4) as

$$[(\vec{r}_{12}\vec{r}_{12})_{2q}(\vec{\sigma}_1\vec{\sigma}_2)_{2p}]_{00}=5^{-1/2}\sum_{q}(\vec{r}_{12}\vec{r}_{12})_{2q}(\vec{\sigma}_1\vec{\sigma}_2)^{\dagger}_{2q}\,. \tag{5}$$

The spin part of the tensor interaction (2) is already separated in the spin coordinates of the two particles, while the space part $V(r_{12})(\vec{r}_{12}\vec{r}_{12})_{2q}$ depends explicitly on the relative position of the two particles. Because in a central-field approximation the space eigenfunction of particle $i$ depends only on its own coordinates $\vec{r}_i$, the evaluation of matrix elements will become considerably simpler if we manage to separate the space part into a product of functions of the individual coordinates $\vec{r}_1$ and $\vec{r}_2$. This can be achieved to the extent that the angular coordinates $\Omega_1$ and $\Omega_2$ are separated.

We note that $V(r_{12})(\vec{r}_{12}\vec{r}_{12})_{2q}$ transforms like an irreducible tensor of rank 2 and can therefore be expanded in a complete orthonormal set of tensors of the form

$$T_{2q}(j'j)=\sum_{m',m}\langle j'm'jm\,|2q\rangle Y_{j'm'}(\Omega_1)Y_{jm}(\Omega_2)\,, \tag{6}$$

where $Y_{jm}$ are the spherical harmonics. Such an expansion would enable a straightforward evaluation of the $m$-scheme matrix element using angular-momentum eigenstates. The expansion is obtained as

$$V(r_{12})(\vec{r}_{12}\vec{r}_{12})_{2q}=\sum_{j'j}C(j'j)T_{2q}(j'j)\,, \tag{7}$$

with the radial coefficients $C(j'j)$ given by

$$C(j-2,j)=(-)^j\left(\frac{j(j-1)}{5(2j-1)}\right)^{1/2}\times(r_1^2V_j+r_2^2V_{j-2}-2r_1r_2V_{j-1})\,, \tag{8a}$$

$$C(j,j)=(-)^{j+1}\left(\frac{2j(j+1)}{15(2j-1)(2j+1)(2j+3)}\right)^{1/2}\times\{(2j+1)(r_1^2+r_2^2)V_j-r_1r_2[(2j-1)V_{j+1}+(2j+3)V_{j-1}]\}\,, \tag{8b}$$

$$C(j+2,j)=(-)^j\left(\frac{(j+1)(j+2)}{5(2j+3)}\right)^{1/2}\times(r_1^2V_j+r_2^2V_{j+2}-2r_1r_2V_{j+1})\,. \tag{8c}$$

Here the radial functions $V_l$ are defined by the generalized Laplace expansion[18]

$$V(r_{12})=\sum_{lm}V_l(r_1r_2)Y^*_{lm}(\Omega_1)Y_{lm}(\Omega_2) \tag{9}$$

for any well-behaved function $V(r_{12})$; many expansions of this type are well known and converge fast.

To summarize the results obtained in this section we present the spherical tensor expansion of the tensor interaction (2) as

$$V_T=5^{-1/2}\sum_{j',j,q}C(j'j)T_{2q}(j'j)(\vec{\sigma}_1\vec{\sigma}_2)^{\dagger}_{2q}\,, \tag{10}$$

with $j'=j,\ j\pm 2$. Compared with other expansions, notably that of Talmi,[13] the present derivation is simple and straightforward and gives a considerably more concise expression. The computational advantage of the present expansion (10) lies in the fact that the dynamical effects of the tensor force are all absorbed in one factor $C(j'j)$ with one recoupling coefficient to be evaluated in calculating many-particle matrix elements.

## III. *m*-SCHEME MATRIX ELEMENT

Matrix elements of a two-particle operator between any many-particle configurations can always be expressed as a linear combination of matrix elements for corresponding two-particle configurations. Consequently we will deal only with the general matrix element for two-particle configurations in the $m$ scheme.

The orbital of a particle has the form

$$|a\rangle\equiv|n_al_am_a\rangle\,|s_a\mu_a\rangle\,, \tag{11a}$$

where $|n_al_am_a\rangle$ and $|s_a\mu_a\rangle$ are the eigenstates of the orbital and spin angular momenta, respectively. Or we can write (11a) explicitly as

$$\psi_{n_a l_a m_a \mu_a} = \frac{1}{r} P_{n_a l_a}(r) Y_{l_a m_a}(\Omega) \chi_{\mu_a}\,, \tag{11b}$$

where $\chi_{\mu_a}$ denotes the spin eigenstate with $s_z = \mu_a$. We emphasize again that the correlation part involving the interparticle distance $r_{12}$ is to be included in the tensor interaction. The $m$-scheme matrix element of the tensor interaction (2) is defined as

$$\langle ab|V_T|cd\rangle = 5^{-1/2} \sum_q \langle n_a l_a m_a(1) n_b l_b m_b(2)\,|V(r_{12})(\vec{r}_{12}\vec{r}_{12})_{2q}|\,n_c l_c m_c(1) n_d l_d m_d(2)\rangle$$
$$\times \langle s_a \mu_a(1) s_b \mu_b(2)\,|(\vec{\sigma}_1\vec{\sigma}_2)^{\dagger}_{2q}|\,s_c \mu_c(1) s_d \mu_d(2)\rangle\,. \tag{12}$$

In order to show later explicitly the coupling of spin angular momenta, we use $s_a$, $s_b$, $s_c$, and $s_d$ instead of their numerical value $\frac{1}{2}$. It is straightforward to express (12) in terms of radial integrals using the expansion (10), and the result is given as

$$\langle ab|V_T|cd\rangle = \sum_{j'j} G_{j'j}(ab;cd) X_{j'j}(ab;cd)\,. \tag{13}$$

In (13) the interaction strength $X_{j'j}(ab;cd)$ is

$$X_{j'j}(ab;cd) = \frac{3}{2\pi}(-)^{l_a+l_b}[5(2j'+1)(2j+1)(2l_a+1)(2l_b+1)(2l_c+1)(2l_d+1)]^{1/2}$$
$$\times \begin{pmatrix} l_a & j' & l_c \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_b & j' & l_d \\ 0 & 0 & 0 \end{pmatrix} \langle P_a P_b C(j'j) P_c P_d\rangle\,, \tag{14}$$

with the radial integral defined as

$$\langle P_a P_b C(j'j) P_c P_d\rangle = \int_0^\infty dr_1 \int_0^\infty dr_2\, P_{n_a l_a}(r_1) P_{n_b l_b}(r_2) C(j'j) P_{n_c l_c}(r_1) P_{n_d l_d}(r_2)\,. \tag{15}$$

The geometrical factor $G_{j'j}(ab;cd)$ in (13) is given as

$$G_{j'j}(ab;cd) = \sum_{qmm'MM'} \begin{pmatrix} 1 & 1 & 2 \\ m & m' & q \end{pmatrix} \begin{pmatrix} j & j & q \\ M' & M & 2 \end{pmatrix} \begin{pmatrix} s_a & m & \mu_c \\ \mu_a & 1 & s_c \end{pmatrix} \begin{pmatrix} s_b & m' & \mu_d \\ \mu_b & 1 & s_d \end{pmatrix} \begin{pmatrix} l_a & M' & m_c \\ m_a & j' & l_c \end{pmatrix} \begin{pmatrix} l_b & M & m_d \\ m_b & j & l_d \end{pmatrix}. \tag{16}$$

Here, to better indicate the tensor properties of the matrix element, we use the Wigner 3-$j$ symbol in the covariant notation[19] with a modified phase factor.[16] This covariant vector-coupling coefficient, called *the covariant 3-jm symbol* or simply the *3-jm symbol*, is related to the Wigner 3-$j$ symbol[19,20] and the Clebsch-Gordan coefficient[17,20] by

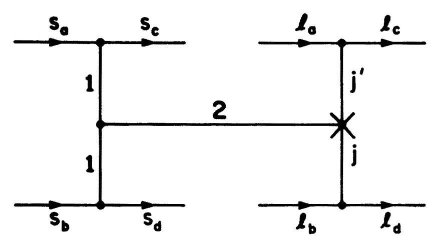
$$\begin{pmatrix} j_1 & j_2 & m_3 \\ m_1 & m_2 & j_3 \end{pmatrix} = (-)^{j_3+m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}$$
$$= (-)^{j_1-j_2-j_3}(2j_3+1)^{-1/2}\langle j_1 m_1 j_2 m_2 | j_3 m_3\rangle\,, \tag{17}$$

where in this particular case the first two components are covariant, and the last component is contravariant. To transform the 3-$jm$ symbol to the Wigner 3-$j$ symbol, we associate each contravariant component $j$ with a phase factor $(-)^{j+m}$ and change the sign of $m$. By this definition the Wigner 3-$j$ symbol is a fully covariant 3-$jm$ symbol.

## IV. GRAPHICAL REPRESENTATION AND APPLICATIONS

With the $m$-scheme matrix element (13) of two-particle configurations, matrix elements between arbitrary many-particle configurations in any coupling scheme can be obtained easily by using computers. For an analytical study of the matrix element, however, it is desirable to obtain an expression in terms of $3n$-$j$ symbols and radial integrals. The complexity in the reduction of angular-momentum couplings can be obviated by adopting a graphical method.[16] The graphical representation of (13) is given as

$\langle ab|V_T|cd\rangle$

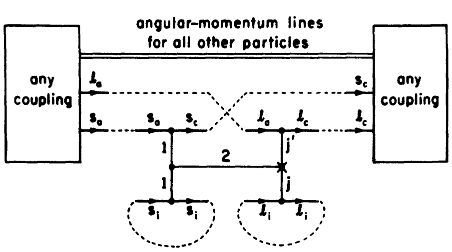
= 

, (18)

where the interaction strength $X_{j'j}(ab;cd)$ and summations over it are denoted by the cross "$X$" at the node $(j'2j)$. In (18) each node represents a $3$-$jm$ symbol, and the three angular-momentum lines originating at the node specify the three components of the $3$-$jm$ symbol. A linked angular-momentum line also implies the summation over the magnetic quantum number associated with it.

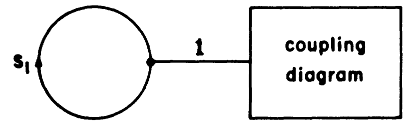
The graphical procedure in evaluating matrix elements between many-particle configurations may be described briefly as follows.[16] By using graphical rules, a many-particle configuration can be constructed as an angular-momentum coupling diagram with the allowance for antisymmetrization. The interaction diagram (18) is then combined with the two diagrams representing the two interacting configurations to form a single angular-momentum diagram. This resulting diagram can be decoded as a sum of products of $3n$-$j$ symbols by using simple graphical rules. Matrix elements between many-particle configurations can thus be expressed as a sum of weighted radial integrals.

As a simple demonstration, we prove graphically that the tensor interaction between a closed shell and arbitrary open shells vanishes. The direct contribution of the many-particle matrix element concerned is given by the diagram



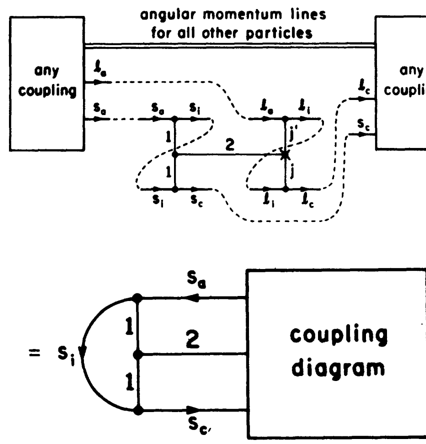

, (19)

where the summation over the closed shell $i$ is performed graphically by joining the corresponding angular-momentum lines $s_i$ and $l_i$. This contribution vanishes because of the fact that




$=0.$ (20)

The exchange contribution is




$=0.$ (21)

The vanishing of this contribution follows from the fact that $s_a(=\frac{1}{2})$, 2, and $s_c$ $(=\frac{1}{2})$ do not satisfy the selection rule of angular-momentum coupling. Therefore we conclude that the tensor interaction between a closed shell and arbitrary open shells vanishes. In fact, this result can readily be seen by inspecting how the angular-momentum lines $s_i$ should be joined together in the $m$-scheme matrix element without drawing the entire recoupling diagram. These and many other similar analyses of different contributions to the tensor interaction in a many-particle system can be carried out easily and expediently.

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