An efficient approach for spin-angular integrations in atomic structure calculations

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Abstract

A general method is described for finding algebraic expressions for matrix elements of any one- and two-particle operator for an arbitrary number of subshells in an atomic configuration, requiring neither coefficients of fractional parentage nor unit tensors. It is based on the combination of second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique. The latter allows us to calculate graphically the irreducible tensorial products of the second quantization operators and their commutators, and to formulate additional rules for operations with diagrams. The additional rules allow us to find graphically the normal form of the complicated tensorial products of the operators. All matrix elements (diagonal and non-diagonal with respect to configurations) differ only by the values of the projections of the quasispin momenta of separate shells and are expressed in terms of completely reduced matrix elements (in all three spaces) of the second quantization operators. As a result, it allows us to use standard quantities uniformly for both diagonal and off-diagonal matrix elements.
1 Introduction

In order to obtain accurate values of atomic quantities it is necessary to account for relativistic and correlation effects. Relativistic effects may be taken into account as Breit-Pauli corrections or, in a fully relativistic approach, by starting with the Dirac-Coulomb Hamiltonian and wave functions defined in terms of four-component one-electron orbitals. In both cases, correlation effects may be considered either variationally or perturbatively. For complex atoms and ions, a considerable part of the effort must be devoted to coping with integrations over spin-angular variables, occurring in the matrix elements of the operators under consideration.

Many existing codes for integrating the spin-angular parts of matrix elements (Glass 1978, Glass and Hibbert 1978, Grant 1988, Burke et al 1994) are based on the computational scheme proposed by Fano (1965). In essence, it consists of evaluating recoupling matrices. Although such an approach uses Racah algebra, it may be necessary to carry out multiple summations over intermediate terms. Due to these summations and the complexity of the recoupling matrix itself, the associated computer codes become rather time consuming. A solution to this problem was found by Burke et al (1994). They tabulated separate standard parts of recoupling matrices along with coefficients of fractional parentage at the beginning of a calculation and used them further on to calculate the needed coefficients. Computer codes by Glass (1978), Glass and Hibbert (1978), Grant (1988), Burke et al (1994) utilize the program NJSYM (Burke 1970) or NJGRAF (Bar-Shalom and Klapisch 1988) for the calculation of recoupling matrices. Both are rather time consuming when calculating matrix elements of complex operators or electronic configurations with many open subshells.

In order to simplify the calculations, Cowan (1981) suggested that matrix elements be grouped into "Classes" (see Cowan 1981 Figure 13-5). Unfortunately, this approach was not generalized to all two-electron operators. Perhaps for this reason Cowan’s approach is not widely used although the program itself, based on this approach is widely used.

Many approaches for the calculation of spin-angular coefficients (Glass 1978, Glass and Hibbert 1978, Grant 1988, Burke et al 1994) are based on the usage of Racah algebra only on the level of coefficients of fractional parentage. A few authors (Jucys and Savukynas 1973, Cowan 1981) utilize the unit tensors, simplifying the calculations in this way, because use can be made of the tables of unit tensors and selection rules can be used to check whether the spin-angular coefficients are zero prior to computation. Moreover, the recoupling matrices themselves have a simpler form. Unfortunately, these ideas were applied only to diagonal matrix elements with respect to configurations, though Cowan (1981) suggested the usage of unit tensors for non-diagonal ones as well.

All the above mentioned approaches were applied in the coordinate representation. The second quantization formalism (Judd 1967, Rudzikas and Kaniauskas 1984, Rudzikas 1991 and Rudzikas 1997) has a number of advantages compared to coordinate representation. First of all, it is much easier to find algebraic expressions for complex operators and their matrix elements, when relying on second quantization formalism. It has contributed significantly to the successful development of perturbation theory (see Lindgren and Morrison 1982, Merkelis et al 1985), and orthogonal operators (Uylings 1984), where three-particle operators already occur. Uylings (1992) suggested a fairly simple approach for dealing with separate cases of three-particle operators. Moreover, in the second quantization approach the quasispin formalism was efficiently developed by Rudzikas and Kaniauskas (1984). The main advantage of this approach is that applying the quasispin method for calculating the matrix elements of any operator, we can use the reduced coefficients of fractional parentage whose matrix elements are independent of the occupation number of the shell. All this enabled Merkelis and Gaigalas (1985) to work out a general perturbation theory approach for complex cases of several open shells.
Thus, it seems that it is possible to formulate an efficient and general approach for finding the spin-angular parts of matrix elements of atomic interactions, relying on the combination of the second quantization approach in the coupled tensorial form, the generalized graphical technique and angular momentum theory in orbital, spin and quasispin spaces as well as the symmetry properties of the quantities considered, which would be free of previous shortcomings. Gaigalas and Rudzikas (1996) suggested such an approach for finding matrix elements of any one- and two-particle atomic operator for the case of two open shells of equivalent electrons. But the situation is different when the matrix elements between more complex configurations are considered.

An approach for the latter case is described in the present paper. One of the main ideas proposed here allows one to solve the problems related to the more complex configurations. Namely, we propose to apply Wick’s theorem (see Lindgren and Morrison 1982) not in its usual general form while calculating the matrix elements, but rather only for groups of operators acting upon distinct shells of equivalent electrons. So, the ordering of operators generally would not be normal.

It is a universal approach for finding algebraic expressions for matrix elements of any one- and two-particle operator in the general case of an arbitrary number of subshells in an atomic configuration, heavily based on the exploitation of the quasispin technique and of the Wigner-Eckart theorem in quasispin space. Expressions for matrix elements and recoupling matrices are obtained by first classifying each matrix element into one of four classes, depending on the number of subshells being acted upon. Each class is then further subdivided into cases and explicit expressions derived for each case in terms of triangular conditions, $nj$-symbols, and reduced matrix elements. From these expressions, efficient procedures can be developed, that apply tests before performing computation.

Tensorial expressions for any two-particle operator are presented in Section 2. They are based on the underlying assumption that the second quantization operators (both creation and annihilation), acting on the same open shell, must always be beside one another in a tensorial product and must be coupled into a resultant momentum. Then the second quantization operators, acting on the next shell, must follow, etc. Section 3 deals with the matrix elements between complex configurations. General expressions for recoupling matrices were found (Section 4) by use of the modified graphical technique of Jucys and Bandzaitis (1977), allowing us to calculate graphically the irreducible tensorial products of the second quantization operators and their commutators, and to formulate additional rules for operations with diagrams. The additional rules allow us to find graphically the normal form of the complicated tensorial products of the operators. All the graphical transformations we use here are fully described in Gaigalas and Rudzikas 1996.

Exploitation of this new version of Racah algebra based on the angular momentum theory, on a generalized graphical approach, on quasispin approach, and on the use of reduced coefficients of fractional parentage for finding the spin-angular parts of two-particle operators is outlined in Sections 5-7. Some details of the calculations are presented in the appendix.

## 2 Tensorial expressions for any two-particle operators

In order to be able to find the expressions for matrix elements of the operators studied, we have to express these operators in terms of the irreducible tensors or their irreducible products. In this section we will present all the necessary tensorial expressions for any two-particle operator $G$.

First, we express the operator in second-quantization form (Gaigalas and Rudzikas 1996) as

$$G = \sum_{n_i,l_i,n_j,l_j,n_i',l_i',n_j',l_j'} \hat{G}(n_i,l_i,n_j,l_j,n_i',l_i',n_j',l_j') = \frac{1}{2} \sum_{i,j,i',j'} a_i a_j a_i^\dagger a_j^\dagger (i,j | g | i', j')$$

(1)
where, as is customary, the creation operators \( a_i, a_j \) appear to the left of the annihilation operators \( a_i^\dagger, a_j^\dagger \), before defining the shells upon which the second quantization operators are acting. After defining the shells explicitly, the second quantization operators are transformed using their commutation relations so that all operators with the same \( n\lambda (\lambda = l, s) \) are beside one another. For example, in the case where the electron creation operator \( a_i \), and electron annihilation operators \( a_i^\dagger \) (where \( i \equiv n_i l_i s_{i,m_{i,s_i}} \)) and \( a_j^\dagger \) act upon the same shell \( \alpha \), and operator \( a_j \) acts upon another shell \( \beta \), we have:

\[
\hat{G}(\alpha \beta \alpha) = \frac{1}{2} \sum_{m_{i\alpha},m_{i\beta}} \sum_{m_{j\alpha},m_{j\beta}} \sum_{m_{s\alpha},m_{s\beta}} a_{m_{i\alpha} m_{s\alpha}}^\dagger a_{m_{i\beta} m_{s\beta}} \times
\]

\[
\times (n_{\alpha} \lambda_{\alpha} m_{i\alpha} s_{i,\alpha}, n_{\beta} \lambda_{\beta} m_{i\beta} s_{i,\beta} | g^{(k_1 k_2 k, \sigma_1 \sigma_2 k)} | n_{\alpha} \lambda_{\alpha} m_{i\alpha} s_{i,\alpha}, n_{\alpha} \lambda_{\alpha} m_{i\beta} s_{i,\beta}) \cdot
\]

Here we imply that a tensorial structure indexed by \((k_1 k_2 k, \sigma_1 \sigma_2 k)\) at \( g \) has rank \( k_1 \) for electron 1, rank \( k_2 \) for electron 2, and a resulting rank \( k \) in the \( l \) space, and corresponding ranks \( \sigma_1 \sigma_2 k \) in the \( s \) space.

Now, applying the graphical approach of angular momentum theory (Gaigalas et al. 1985), we can get an expression, namely

\[
\hat{G}(\alpha \beta \alpha) = \frac{1}{2} \sum_{\kappa_{12}} \sum_{\sigma_{12}} \sum_{k} (-1)^{\kappa_{12} + \sigma_{12} - \kappa_{12}' - \sigma_{12}'} \times
\]

\[
\times (n_{\alpha} \lambda_{\alpha} n_{\beta} \lambda_{\beta} | g^{(k_1 k_2 k, \sigma_1 \sigma_2 k)} | n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha}) \times
\]

\[
\times [\kappa_{12}, \sigma_{12}] \left[ | \kappa_{12}', \sigma_{12}' \right]^{1/2} \left\{ \begin{array}{ccc}
\kappa_1 & \kappa_2 & k \\
\kappa_1' & \kappa_2' & k'
\end{array} \right\} \left\{ \begin{array}{ccc}
s & s & \sigma_{12} \\
s & s & \sigma_{12}'
\end{array} \right\} \times
\]

\[
\times \sum_{K_{1s}, K_{s}} [K_{1s}, K_{s}]^{1/2} \left\{ \begin{array}{ccc}
l_1 & l_2 & \kappa_{12} \\
\kappa_{12}' & K_{1s} & K_{s}
\end{array} \right\} \left\{ \begin{array}{ccc}
s & s & \sigma_{12} \\
s & s & \sigma_{12}'
\end{array} \right\} \times
\]

\[
\times \left[ a(l_{1s}) \times a(l_{2s}) \times a(l_{2s})^\dagger \times a(l_{1s})^\dagger \right]_{p,-p}^{(kk)}
\]

where \([a, b] = (2a + 1)(2b + 1)\), \((n_{\alpha} \lambda_{\alpha} n_{\beta} \lambda_{\beta} | g^{(k_1 k_2 k, \sigma_1 \sigma_2 k)} | n_{\alpha} \lambda_{\alpha} n_{\alpha} \lambda_{\alpha})\) is the two-electron submatrix (reduced matrix) element of operator \( \hat{G} \) and \( a(l_{1s})^\dagger \) is defined as (Judd 1967)

\[
a(l_{1s})^\dagger a(m_{1s}, m_{s}) = (-1)^{l_1 + s - m_{s} - m_{s}} a(l_{1s}) a(l_{1s})^\dagger.
\]

Expression (3) has summations over intermediate ranks \( \kappa_{12}, \sigma_{12}, K_{1s}, K_{s} \) in tensorial product. The angular momentum projection of \((kk)\) is \( p, -p \).

In order to calculate the spin-angular part of a two-particle operator matrix element with an arbitrary number of open shells, it is necessary to consider all possible distributions of subshells, upon which the second quantization operators are acting. These are presented in Table 1. We point out that for distributions 2–5 and 19–42 the shells' sequence numbers \( \alpha, \beta, \gamma, \delta \) (in bra and ket functions of a submatrix element) satisfy the condition \( \alpha < \beta < \gamma < \delta \), while for distributions 6–18 no conditions upon \( \alpha, \beta, \gamma, \delta \) are imposed.
Table 1: Distributions of subshells, upon which the second quantization operators are acting, that appear in
the submatrix elements of any two-particle operator, when bra and ket functions have $u$ open subshells

| No. | $a_i$ | $a_j$ | $a_i^\dagger$ | $a_j^\dagger$ | submatrix element |
|-----|-------|-------|---------------|---------------|------------------|
| 1.  | $\alpha$ | $\alpha$ | $\alpha$ | $\alpha$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\alpha l_{N_\alpha}^N \ldots$ |
| 2.  | $\alpha$ | $\beta$ | $\alpha$ | $\beta$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\beta l_{N_\beta}^N \ldots$ |
| 3.  | $\beta$ | $\alpha$ | $\beta$ | $\alpha$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\alpha l_{N_\alpha}^N \ldots$ |
| 4.  | $\alpha$ | $\beta$ | $\beta$ | $\alpha$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\beta l_{N_\beta}^N \ldots$ |
| 5.  | $\beta$ | $\alpha$ | $\alpha$ | $\beta$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\alpha l_{N_\alpha}^N \ldots$ |
| 6.  | $\alpha$ | $\alpha$ | $\beta$ | $\beta$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\alpha l_{N_\alpha}^N \ldots \ldots n_\beta l_{N_\beta}^N \ldots$ |
| 7.  | $\beta$ | $\alpha$ | $\alpha$ | $\alpha$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\alpha l_{N_\alpha}^N \ldots$ |
| 8.  | $\alpha$ | $\beta$ | $\alpha$ | $\alpha$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\beta l_{N_\beta}^N \ldots$ |
| 9.  | $\beta$ | $\beta$ | $\alpha$ | $\alpha$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\alpha l_{N_\alpha}^N \ldots$ |
| 10. | $\beta$ | $\alpha$ | $\alpha$ | $\beta$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_\alpha l_{N_\alpha}^N \ldots$ |
| 11. | $\beta$ | $\gamma$ | $\alpha$ | $\gamma$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 12. | $\gamma$ | $\beta$ | $\gamma$ | $\alpha$ | $\ldots n_\gamma l_{N_\gamma}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\beta l_{\beta}^N \ldots$ |
| 13. | $\gamma$ | $\beta$ | $\alpha$ | $\gamma$ | $\ldots n_\gamma l_{N_\gamma}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\alpha l_{\alpha}^N \ldots$ |
| 14. | $\beta$ | $\gamma$ | $\gamma$ | $\alpha$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\alpha l_{\alpha}^N \ldots$ |
| 15. | $\gamma$ | $\gamma$ | $\alpha$ | $\beta$ | $\ldots n_\gamma l_{N_\gamma}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 16. | $\gamma$ | $\gamma$ | $\beta$ | $\alpha$ | $\ldots n_\gamma l_{N_\gamma}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 17. | $\alpha$ | $\beta$ | $\gamma$ | $\gamma$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 18. | $\beta$ | $\alpha$ | $\gamma$ | $\gamma$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 19. | $\alpha$ | $\beta$ | $\gamma$ | $\delta$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 20. | $\beta$ | $\alpha$ | $\gamma$ | $\delta$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 21. | $\alpha$ | $\beta$ | $\delta$ | $\gamma$ | $\ldots n_\alpha l_{N_\alpha}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
| 22. | $\beta$ | $\alpha$ | $\delta$ | $\gamma$ | $\ldots n_\beta l_{N_\beta}^N \ldots | G(n_{i\gamma} l_{j\gamma} n_{i\gamma}^l n_{j\gamma}^l) | \ldots n_{\gamma l_{\gamma}^N \ldots$ |
Let $\Xi$ be an array of intermediate coupling parameters in tensorial form, including $\kappa_{12}, \sigma_{12}, \kappa_{12}', \sigma_{12}'$ and possibly also others. Then the tensorial expressions for all these distributions can be grouped into four classes, where in each class, the two-particle operator $\tilde{G}$, operating on specific shells (see Eq. (1)), has one of four forms:

1. All the second quantization operators act upon the same shell (distribution 1) and

$$\tilde{G}(I) \sim \sum_{\kappa_{12}, \sigma_{12}, \kappa_{12}', \sigma_{12}'} \sum_{\mathbf{p}} \Theta(n_\lambda, \Xi) A_{\mathbf{p}, \mathbf{p}'}^{(kk)} (n_\lambda, \Xi);$$

2. The second quantization operators act upon the two different shells (distributions 2-10) and

$$\tilde{G}(II) \sim \sum_{\kappa_{12}, \sigma_{12}, \kappa_{12}', \sigma_{12}'} \sum_{\mathbf{p}} \Theta(n_\lambda n_\kappa, \Xi) \times
\left[ B^{(\kappa_{12} \sigma_{12})} (n_\alpha, \Xi) \times C^{(\kappa_{12}' \sigma_{12}')} (n_\beta, \Xi) \right]_{\mathbf{p}, \mathbf{p}'}^{(kk)};$$

3. The second quantization operators act upon three shells (distributions 11-18)
\[ \hat{G} (III) \sim \sum_{\kappa_1, \sigma_1, \kappa_2, \sigma_2} \sum_{p} \Theta (n_\alpha \lambda_\alpha, n_\beta \lambda_\beta, n_\gamma \lambda_\gamma, \Xi) \times \]
\[ \times \left[ D(l_1, s_1) \times D(l_3, s_3) \right] (\kappa_1 \sigma_1 \kappa_2 \sigma_2) \times E(\kappa_2 \sigma_2 \kappa_3 \sigma_3) (n_\gamma \lambda_\gamma, \Xi) \right]^{(kk)}_{p, -p} ; \]  

(7)

4. The second quantization operators act upon four shells (distributions 19-42) and

\[ \hat{G} (IV) \sim \sum_{\kappa_1, \sigma_1, \kappa_2, \sigma_2} \sum_{p} \Theta (n_\alpha \lambda_\alpha, n_\beta \lambda_\beta, n_\gamma \lambda_\gamma, n_\delta \lambda_\delta, \Xi) \times \]
\[ \times \left[ D(l_1, s_1) \times D(l_3, s_3) \right] (\kappa_1 \sigma_1 \kappa_2 \sigma_2) \times \left[ D(l_3, s_3) \times D(l_4, s_4) \right] (\kappa_2 \sigma_2 \kappa_3 \sigma_3) \right]^{(kk)}_{p, -p} . \]

(8)

In (5)-(8), \( \Theta (n_\lambda \Xi) \), ..., \( \Theta (n_\alpha \lambda_\alpha, n_\beta \lambda_\beta, n_\gamma \lambda_\gamma, n_\delta \lambda_\delta, \Xi) \) are proportional to the radial part of the operator \( \hat{G} \), and \( A^{(kk)} (n_\lambda \Xi) \), ..., \( E^{(kk)} (n_\lambda \Xi) \) denote tensorial products of irreducible tensors. Parameter \( \Xi \) implies the array of coupling parameters that connect \( \Theta \) to the tensorial part. The explicit tensorial expressions are presented in the Appendix, using the graphical approach of Gaigalas et al (1985). Graphical methods make it possible to reduce the number of expressions from 42 to 6 for all distributions presented in Table 1. Such a joining up of several distributions is possible by graphical methods, because in the graphical technique of Jucys and Bandzaitis (1977), as in the tensorial products of operators of second quantization, the main elements are the Clebsch-Gordan coefficients. Therefore we may join up all the distributions having essentially the same algebraic structure, although with different tensorial products. The latter are represented by diagrams in which all the peculiarities of a tensorial product are seen, and the differences of particular distributions are easily noticed. The use of other graphical methods (see e.g. Yutis et al 1962 or Lindgren and Morrison 1982) in joining up the distributions is complicated, since there the Wigner coefficients play the main role, and these are not fully compatible with the graphical transformations of the operators of second quantization in coupled form. Having classified the operators, we will now consider matrix elements of these operators for arbitrary configurations.

### 3 Matrix elements between complex configurations

Now, having the irreducible tensorial form of the operator being considered, we are in a position to find their matrix elements and recoupling matrices. Suppose that we have a bra function with \( u \) shells in \( LS \) coupling:

\[ \psi_u^{\text{bra}} (LSM_L M_S) \equiv \]
\[ \equiv (n_1 l_1 n_2 l_2 \ldots n_u l_u \alpha_1 L_1 S_1 Q_1 M_Q_1 \alpha_2 L_2 S_2 Q_2 M_Q_2 \ldots \alpha_u L_u S_u Q_u M_Q_u A L S M_L M_S) \]  

(9)

and a ket function:

\[ \psi_u^{\text{ket}} (L'S'M_L'M_S') \equiv \]
\[ \equiv |n_1 l_1 n_2 l_2 \ldots n_u l_u \alpha_1' L_1' S_1' Q_1' M_Q_1 \alpha_2' L_2' S_2' Q_2' M_Q_2 \ldots \alpha_u' L_u' S_u' Q_u' M_Q_u A' L' S' M_L'M_S') \]  

(10)

where \( A \) stands for all intermediate quantum numbers, depending on the order of coupling of momenta \( L_i S_i \). Label \( Q_i \) is the quasispin momentum of the shell \( n_i l_i \), which is related to the seniority quantum number \( \nu_i \), namely, \( Q_i = (2l_i + 1 - \nu_i) / 2 \), and its projection, \( M_Q_i = (N_i - 2l_i - 1) / 2 \). In (9) and (10) \( \alpha_i \) denotes all additional quantum numbers needed for the classification of the energy levels of the relevant shell.

Using the Wigner-Eckart theorem in \( LS \) space we shift from the matrix element of any two-particle operator \( G \) between functions (9) and (10) to the submatrix element \( \langle \psi_u^{\text{bra}} (LS) | G | \psi_u^{\text{ket}} (L'S') \rangle \) of this operator.
A general expression for the submatrix element of any two-particle operator between functions (9) and (10) with \( u \) open shells can be written as

\[
\langle \psi_u^{\text{bra}} | (LS) | G | \psi_u^{\text{ket}} (L'S') \rangle = \sum_{n_i,l_i,n_j,l_j,n_i',l_i',\kappa_{12},\sigma_{i2}} \sum_{i,j} (-1)^{\Delta} \Theta' (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j') \times \\
\times T (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}, \Xi, \Gamma}) \times \\
\times R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}, \Gamma})
\]

where \( \Lambda^{\text{bra}} \equiv (L_i S_i, L_j S_j, L_i' S_i', L_j' S_j')^{\text{bra}} \) is the array for the bra function shells’ terms, and similarly for \( \Lambda^{\text{ket}} \). This expression is similar to Eq. (136) used by Grant (1988) in his derivation. So, to calculate the spin-angular part of a submatrix element, one has to compute:

1. The recoupling matrix \( R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}, \Gamma}) \). This recoupling matrix accounts for the change in going from matrix element \( \langle \psi_u^{\text{bra}} | (LS) | G | \psi_u^{\text{ket}} (L'S') \rangle \), which has \( u \) open shells in the bra and ket functions, to the submatrix element \( T (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}, \Xi, \Gamma}) \), which has only the shells being acted upon by the two-particle operator in its bra and ket functions.

2. The submatrix element \( T (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}, \Xi, \Gamma}) \), which denotes the submatrix elements of operators of the types \( A^{(kk')}(n, \lambda, \Xi) \), \( B^{(k'k)}(n, \lambda, \Xi) \), \( C^{(kk')}(n, \lambda, \Xi) \), \( D^{(1s)} \), \( E^{(kk')}(n, \lambda, \Xi) \) (see (5)-(8)). Here \( \Gamma \) refers to the array of coupling parameters connecting the recoupling matrix \( R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}, \Gamma}) \) to the submatrix element.

3. Phase factor \( \Delta \).

4. \( \Theta' (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Xi) \), which is proportional to the radial part and corresponds to one of \( \Theta (n_\alpha \lambda_\alpha, \ldots, \Xi) \). It consists of a submatrix element

\[
(n_i \lambda_i n_j \lambda_j | g^{(\kappa_1, \kappa_2, \sigma_2 \sigma_2)} | n_i' \lambda_i' n_j' \lambda_j')
\]

and in some cases of simple factors and \( 3n_j \)-coefficients. For distributions \( \alpha \beta \gamma \alpha \beta, \gamma \gamma \beta \alpha, \alpha \beta \gamma \alpha, \beta \alpha \gamma \gamma, \alpha \beta \gamma \delta, \beta \alpha \gamma \delta, \gamma \delta \beta \alpha, \gamma \delta \beta \alpha, \delta \gamma \beta \alpha, \alpha \beta \gamma \delta \) (see expressions (52), (53) and notes on \( \Theta' \), \( \Theta \) in Appendix) it is:

\[
\Theta' (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Xi) = (-1)^t \tilde{\Theta} (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j') \times \\
\times [\kappa_{12}, \sigma_{12}, \kappa_{12}', \sigma_{12}']^{1/2} \left\{ \begin{array}{ccc} l_i & l_i' & \kappa_1 \\ l_j & l_j' & \kappa_2 \\ \kappa_{12} & \kappa_{12}' & k \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_1 \\ s & s & \sigma_2 \\ \sigma_{12} & \sigma_{12}' & k \end{array} \right\},
\]

where the integer \( t \) determining the phase depends upon the configuration states involved. Rules for its determination are given in the Appendix.

The calculation of \( \Theta' (n_i \lambda_i, n_j \lambda_j, n_i' \lambda_i', n_j' \lambda_j', \Xi) \) is straightforward (from an angular momentum point of view) and depends on the radial form of the operator. In the next sections we will describe expressions for the recoupling matrix, the submatrix elements, and the phase factor, respectively.

### 4 Recoupling matrices

In this section we present the expressions for the recoupling matrices

\[
R (\lambda_i, \lambda_j, \lambda_i', \lambda_j', \Lambda^{\text{bra}}, \Lambda^{\text{ket}, \Gamma}).
\]
These matrices may be treated in the orbital $l$ and spin $s$ spaces separately. That is,

$$
R (\lambda_i, \lambda_j, \lambda'_i, \lambda'_j, A^bra_a, A^ket_b, \Gamma) =
R (l_i, l_j, l'_i, l'_j, A^bra_a, A^ket_b, \Gamma_i) R (s, s, s, s, A^bra_a, A^ket_b, \Gamma_s)
$$

where $A^bra_a \equiv (L_i, L_j, L'_i, L'_j)^{bra_a}$ and $A^bra_s \equiv (S_i, S_j, S'_i, S'_j)^{bra_s}$. Therefore for simplicity we present only the expressions in $l$ space. The recoupling matrices in $s$ space are easily obtained from analogous expressions in $l$ space by making corresponding substitutions $l_1, l_2, ..., l_a \rightarrow s$; $L_1 \rightarrow S_1, L_2 \rightarrow S_2; ..., L_{12} \rightarrow S_{12}; ..., L_{123} \rightarrow S_{123}; ... L \rightarrow S, L' \rightarrow S'$. Also, the analytical expressions for recoupling matrices presented in this section are valid in the case of $jj$-coupling.

As we have mentioned earlier, there are four classes as defined by Eq.’s (5)-(8). We will consider each class separately. All the expressions presented below are obtained by using the approach of angular momentum theory described by Jucys and Bandzaitis (1977).

### 4.1 One interacting shell

Let us assume that the operators of second quantization act upon shell $a$ as in distribution 1 of Table 1, where $a \equiv \alpha$. Then the recoupling matrix has the expression:

$$
R (l_a, l_a, k) = [L_a]^{-1/2} \delta (L_1, L'_1) \ldots \delta (L_{a-1}, L'_{a-1}) \delta (L_{a+1}, L'_{a+1}) \ldots \delta (L_u, L'_u) \times
$$

$$
\begin{cases}
\delta (L_1, L'_1, k); & \text{for } u = 1 \\
C_1; & \text{for } u = 2 \\
C_1 C_2 (k, a + 1, u - 1) C_3; & \text{for } a < 3, u > 2 \\
\delta (L_{12}, L'_{12}) \ldots \delta (L_{12...a-1}, L'_{12...a-1}) \times C_1 C_2 (k, a + 1, u - 1) C_3; & \text{for } a > 3, a \neq u, u > 2 \\
\delta (L_{12}, L'_{12}) \ldots \delta (L_{12...a-1}, L'_{12...a-1}) C_3; & \text{for } a = u, u > 2
\end{cases}
$$

In the above, the notation $\delta (L_1, L'_1, k)$ means the triangular condition $|L_1 - L'_1| \leq k \leq L_1 + L'_1$ and

$$
C_1 = (-1)^{\varphi} [L_a, T']^{1/2} \left\{ k \begin{array}{cc} L'_a & L_a \\ J & T \\ T' & T' \end{array} \right\},
$$

where the values of parameters $\varphi, J, T$ and $T'$ present in expression (15) are given in Table 2. The remaining two coefficients are

$$
C_2 (k, k_{min}, k_{max}) = \prod_{i=k_{min}}^{k_{max}} (-1)^{k + L_i + L_{12...i-1} + L'_{12...i-1}} [L_{12...i-1}, L'_{12...i-1}]^{1/2} \times
$$

$$
\begin{array}{c}
\delta (L_{12...i-1}, L'_{12...i-1}) \\
\delta (L_i, L'_i) \\
\delta (L_{12...i}, L'_{12...i})
\end{array}
$$

(16)

and

$$
C_3 = (-1)^{\varphi} [J, T']^{1/2} \left\{ k \begin{array}{cc} J' & J \\ j & T \\ T & T' \end{array} \right\};
$$

(17)
Table 2: Parameters for equation (15)

| $u$ | $a$ | $\varphi$ | $J$ | $T$ | $T'$ |
|-----|-----|------------|-----|-----|------|
| 2   | 1   | $L_1 + 2L_1' - L_2 - L' + k$ | $L_2$, | $L$ | $L'$ |
| 2   | 2   | $L_1 + L + L_2' + k$ | $L_1$ | $L$ | $L'$ |
| $u \neq 2$ | 1 | $L_1 + 2L_1' - L_2 - L_1' + k$ | $L_2$, | $L_{12}$ | $L_{12}'$ |
| $u \neq 2$ | 2 | $L_1 + L_{12} + L_2' + k$ | $L_1$ | $L_{12}$ | $L_{12}'$ |
| $u \neq 2$ | $a > 2$ | $L_{12...a-1} + L_{12...a} + L_a' + k$ | $L_{12...a-1}$ | $L_{12...a}$ | $L_{12...a}'$ |

Table 3: Parameters for equation (17)

| $u$ | $\varphi$ | $j$ | $J$ | $J'$ | $T$ | $T'$ |
|-----|------------|-----|-----|-----|-----|------|
| $u \neq a$ | $a$ | $k + L_u + L_{12...u-1} + L'$ | $L_u$ | $L_{12...u-1}$ | $L_{12...u-1}'$ | $L$ | $L'$ |
| $a$ | $k - L_{12...u-1} + 2L_u + L_u' - L$ | $L_{12...u-1}$ | $L_u$ | $L_{12...u-1}'$ | $L_u$ | $L'$ |
where the parameters \( \varphi, j, J, J', T \) and \( T' \) are given in Table 3.

When the total rank \( k = 0 \), the recoupling matrix becomes simply

\[
R(l_a, L_a, 0) = \delta(L_1, L'_1) \delta(L_2, L'_2) \delta(L_{a-1}, L'_{a-1}) \times \\
\times \delta(L_{12...a-1}, L'_{12...a-1}) \delta(L_a, L'_a) \delta(L_{a+1}, L'_{a+1}) \times \\
\times \delta(L_{12...a+1}, L'_{12...a+1}) \delta(L_u, L'_u) \delta(L, L').
\]

Expression (18) is equivalent to (13.60) of Cowan (1981).

### 4.2 Two interacting shells

In this case let us assume that the operators of second quantization act upon the shells \( a \) and \( b \) (distributions 2-10 in Table 1, where for distributions 2-5 \( a \equiv \alpha, b \equiv \beta \) and for others (6-10) \( a = \min\{\alpha, \beta\}, b = \max\{\alpha, \beta\} \)). Then

\[
R(l_a, L_a, l_b, L_b, \kappa_{12}, \kappa'_{12}, k) = (-1)^{\zeta} [L_a, L_b]^{-1/2} \delta(L_1, L'_1) \times \\
\times \delta(L_{a+1}, L'_{a+1}) \delta(L_{b-1}, L'_{b-1}) \delta(L_u, L'_u) \times \\
C_4(K_{12}, K'_{12}, k, 1) C_2(k, 3, u - 1) C_3;
\]

\[
\times \left\{ \begin{array}{ll}
C_1 C_2(K_{12}, a + 1, b - 1) C_4(K_{12}, K'_{12}, k, 1) \times \\
\times C_2(k, b + 1, u - 1) C_3; & \text{for } a < 3, b > 2, b \neq u
\end{array} \right.
\]

\[
\times C_1 C_2(K_{12}, a + 1, b - 1) C_4(K_{12}, K'_{12}, k, 1); & \text{for } a < 3, b = u
\]

\[
\times \left\{ \begin{array}{ll}
\delta(L_{12}, L'_{12}) \times \delta(L_{12...a-1}, L'_{12...a-1}) C_1 \times \\
\times C_2(K_{12}, a + 1, b - 1) C_4(K_{12}, K'_{12}, k, 1) \times \\
\times C_2(k, b + 1, u - 1) C_3; & \text{for } a \geq 3, b > 2, b \neq u
\end{array} \right.
\]

\[
\times C_1 C_2(K_{12}, a + 1, b - 1) C_4(K_{12}, K'_{12}, k, 1); & \text{for } a \geq 3, b = u
\]

where

\[
\zeta = \begin{cases}
0 & \text{for } \alpha < \beta, \\
\kappa_{12} + \kappa'_{12} - k & \text{for } \alpha > \beta,
\end{cases}
\]

and

\[
C_4(k_1, k_2, k, P) = |J_1, J_2, J'_3, k|^{1/2} \left\{ \begin{array}{cccc}
J'_1 & k_1 & J_1 \\
J'_2 & k_2 & J_2 \\
J'_3 & k & J_3
\end{array} \right\}.
\]

The values of parameters \( J_1, J'_1, J_2, J'_2, J_3 \) and \( J'_3 \) present in the expression (21) must be taken from Table 4. For the case \( \alpha < \beta \) in Eq. (19) \( K_{12} = \kappa_{12}, K'_{12} = \kappa'_{12} \) and when \( \alpha > \beta \), then \( K_{12} = \kappa'_{12}, K'_{12} = \kappa_{12} \).
Table 4: Parameters for equation (21)

| P |  a  |  b  |  u  |  J_1  |  J'_1  |  J_2  |  J'_2  |  J_3  |  J'_3  |
|---|-----|-----|-----|-------|-------|-------|-------|-------|-------|
| 1 | 1   | 2   | u ≠ b | L_1   | L'_1  | L_2   | L'_2  | L_{12} | L'_{12} |
| 1 | 1   | 2   | b    | L_1   | L'_1  | L_2   | L'_2  | L   | L   |
| 1 | a ≠ 1 | b ≠ 2 | b    | L_{1...u-1} | L'_{1...u-1} | L_u | L'_u | L | L' |
| 1 | in all cases | L_{1...b-1} | L'_{1...b-1} | L_b | L'_b | L_{1...b} | L'_{1...b} |
| 2 | in all cases | L_{1...c-1} | L'_{1...c-1} | L_c | L'_c | L_{1...c} | L'_{1...c} |

When the total rank \( k = 0 \), and \( \kappa_{12} = \kappa'_{12} = k \), the recoupling matrix has the form:

\[
R(l_a, L_a, l_b, L_b, k, k, 0) = [L_a, L'_b, k]^{-1/2} \delta(L_1, L'_1) \cdots \delta(L_{a-1}, L'_{a-1}) \times \\
\times \delta(L_{a+1}, L'_{a+1}) \cdots \delta(L_{b-1}, L'_{b-1}) \delta(L_{b+1}, L'_{b+1}) \delta(L_u, L'_u) \times \\
\times \delta(L_{12}, L'_{12}) \cdots \delta(L_{12...a-1}, L'_{12...a-1}) \delta(L_{12...b}, L'_{12...b}) \cdots \delta(L, L') \\
\]

\[
x \begin{cases}
C_5(1); & \text{for } a = 1, b = 2 \\
C_1C_2(k, a + 1, b - 1) C_5(1); & \text{for } a < 3 \\
\delta(L_{12}, L'_{12}) \cdots \delta(L_{12...a-1}, L'_{12...a-1}) \times C_1C_2(k, a + 1, b - 1) C_5(1); & \text{for } a \geq 3
\end{cases}
\]

where

\[
C_5(P) = (-1)^{k+L_u+J'_1+J_2} [J_1, L'_b]^{1/2} \begin{pmatrix} k & L_b & L_b \\ J_2 & J_3 & J'_1 \end{pmatrix}.
\]

The values of parameters \( J_1, J'_1 \) and \( J_2 \) present in the expression (23) must be taken from Table 5.

Formula (22) has no analogue in Cowan (1981). Our expressions for the recoupling matrix do not depend on coefficients of fractional parentage and have no intermediate summations. Therefore they will be very convenient for practical calculations.

4.3 Three interacting shells

When the operators of second quantization act upon three shells \( a, b \) and \( c \) (distributions 11-18 in the Table 1), we have:
Table 5: Parameters for equation (23)

| P | Case                        | $J_1$     | $J'_1$    | $J_2$     |
|---|-----------------------------|-----------|-----------|-----------|
| 1 | $a = 1$ and $b = 2$         | $L_a$     | $L'_a$    | $L_{12...b}$ |
| 1 | $b \neq u$                  | $L_{1...b-1}$ | $L'_{1...b-1}$ | $L_{12...b}$ |
| 1 | $b = u$                     | $L_{1...b-1}$ | $L'_{1...b-1}$ | $L$        |
| 2 | $c \neq u$                  | $L_{1...c-1}$ | $L'_{1...c-1}$ | $L_{12...c}$ |
| 2 | $c = u$                     | $L_{1...c-1}$ | $L'_{1...c-1}$ | $L$        |
| 3 | $d \neq u$                  | $L_{1...d-1}$ | $L'_{1...d-1}$ | $L_{12...d}$ |
| 3 | $d = u$                     | $L_{1...d-1}$ | $L'_{1...d-1}$ | $L$        |

From (7) we have that in expressions (24) and (25) the ranks $k_1 = l_a$, $k_2 = l_b$. 

\[
\begin{align*}
R(l_a, l_a, l_b, l_b, l_c, l_c, k_1, k_2, \kappa_{12}, \kappa'_{12}, k) &= \\
&= [l_a, l_b, l_c]^{-1/2} \delta (L_1, L_1') \cdots \delta (L_{a-1}, L'_{a-1}) \times \\
&\times \delta (L_{a+1}, L'_{a+1}) \cdots \delta (L_{b-1}, L'_{b-1}) \delta (L_{b+1}, L'_{b+1}) \cdots \delta (L_{c-1}, L'_{c-1}) \times \\
&\times \delta (L_{c+1}, L'_{c+1}) \delta (L_u, L'_u) \sum_{j=12} (-1)^j C_6 \times \\
&\times C_4(K_1, K_2, j_{12}, 1) C_2(j_{12}, 3, c - 1) \times \\
&\times C_4(j_{12}, K_3, k, 2) C_2(k, c + 1, u - 1) C_3; \quad \text{for } a = 1, b = 2 \\
&\times C_1 C_2(K_1, a + 1, b - 1) C_4(K_1, K_2, j_{12}, 1) \times \\
&\times C_2(j_{12}, b + 1, c - 1) C_4(j_{12}, K_3, k, 2) \times \\
&\times C_2(k, c + 1, u - 1) C_3; \quad \text{for } a < 3 \\
&\times \delta (L_{12}, L'_{12}) \cdots \delta (L_{12...a-1}, L'_{12...a-1}) C_1 \times \\
&\times C_2(K_1, a + 1, b - 1) C_4(K_1, K_2, j_{12}, 1) \times \\
&\times C_2(j_{12}, b + 1, c - 1) C_4(j_{12}, K_3, k, 2) \times \\
&\times C_2(k, c + 1, u - 1) C_3; \quad \text{for } a \geq 3,
\end{align*}
\]

where parameters $a$, $b$, $c$, $\zeta$, $K_1$, $K_2$, $K_3$ and coefficient $C_6$ are given in Table 6. The coefficient $C_6(k_1, k_2, k_3, k_4, k_5, k_6)$ is

\[
C_6(k_1, k_2, k_3, k_4, k_5, k_6) = (-1)^{k_1+k_2-k_3+2k_5} [k_3, k_6]^{1/2} \left\{ \begin{array}{ccc} k_1 & k_2 & k_3 \\ k_4 & k_5 & k_6 \end{array} \right\}. \tag{25}
\]
When the total rank $k = 0$, and $\kappa_{12} = \kappa'_{12} = k$, the recoupling matrix has the form:

$$R (l_a, L_a, l_b, L_b, l_c, L_c, k_1, k_2, k, 0) = (-1)^\zeta [L_a, L_b, L'_c, K_3]^{-1/2} \times$$

$$\times \delta (L_1, L'_1) \ldots \delta (L_{a-1}, L'_{a-1}) \delta (L_{a+1}, L'_{a+1}) \ldots \delta (L_{b-1}, L'_{b-1}) \times$$

$$\times \delta (L_{b+1}, L'_{b+1}) \ldots \delta (L_{c-1}, L'_{c-1}) \delta (L_{c+1}, L'_{c+1}) \ldots \delta (L_{u}, L'_{u}) \times$$

$$\times \delta (L_{12}, L'_{12}) \ldots \delta (L_{12-\text{a-1}}, L'_{12-\text{a-1}}) \delta (L_{12-\text{c-1}}, L'_{12-\text{c-1}}) \ldots \delta (L_{L'}, L'_{L'}) \times$$

$$\left\{ \begin{aligned}
& C_4 (K_1, K_2, K_3, 1) C_2 (K_3, b + 1, c - 1) C_5 (2); \quad \text{for } a = 1, b = 2 \\
& C_1 C_2 (K_1, a + 1, b - 1) C_4 (K_1, K_2, K_3, 1) \\
& \times C_2 (K_3, b + 1, c - 1) C_5 (2); \quad \text{for } a < 3 \\
& \delta (L_{12}, L'_{12}) \ldots \delta (L_{12-\text{a-1}}, L'_{12-\text{a-1}}) C_1 \\
& \times C_2 (K_1, a + 1, b - 1) C_4 (K_1, K_2, K_3, 1) \\
& \times C_2 (K_3, b + 1, c - 1) C_5 (2); \quad \text{for } a \geq 3
\end{aligned} \right\}$$

where the parameters $\zeta$, $K_1$, $K_2$, $K_3$ values are given in Table 7.

The recoupling matrix for three interacting shells (26) has the same advantages as the equivalent quantity, Eq. (22), for two shells.

### 4.4 Four interacting shells

When the operators of second quantization act upon four shells $a$, $b$, $c$ and $d$ (distributions 19-42 in the Table 1), we have:
\[ R (l_a, L_a, b, L_b, L_c, l_d, L_d, k_1, k_2, \kappa_{12}, k_3, k_4, \kappa'_{12}, k) = \]
\[ = [L_a, L_b, L_c, L_d]^{-1/2} \delta (L_1, L'_1) \ldots \delta (L_{a-1}, L'_{a-1}) \times \]
\[ \times \delta (L_{a+1}, L'_{a+1}) \ldots \delta (L_{b-1}, L'_{b-1}) \delta (L_{b+1}, L'_{b+1}) \ldots \delta (L_{c-1}, L'_{c-1}) \times \]
\[ \times \delta (L_{c+1}, L'_{c+1}) \ldots \delta (L_{d-1}, L'_{d-1}) \delta (L_{d+1}, L'_{d+1}) \ldots \delta (L_u, L'_u) \times \]
\[ \begin{cases} 
C_4 (k_1, k_2, \kappa_{12}, 1) C_2 (\kappa_{12}, 3, c - 1) C_7 (c, d) \times \\
\times C_2 (k, d + 1, u - 1) C_3; 
\end{cases} \]
\[ \text{for } a = 1, b = 2 \]
\[ \times \begin{cases} 
C_1 C_2 (k_1, a + 1, b - 1) C_4 (k_1, k_2, \kappa_{12}, 1) \times \\
\times C_2 (\kappa_{12}, b + 1, c - 1) C_7 (c, d) \times \\
\times C_2 (k, d + 1, u - 1) C_3; 
\end{cases} \]
\[ \text{for } a < 3 \]
\[ \delta (L_{12}, L'_{12}) \ldots \delta (L_{12 \ldots a-1}, L'_{12 \ldots a-1}) C_1 \times \\
\times C_2 (k_1, a + 1, b - 1) C_4 (k_1, k_2, \kappa_{12}, 1) \times \\
\times C_2 (\kappa_{12}, b + 1, c - 1) C_7 (c, d) \times \\
\times C_2 (k, d + 1, u - 1) C_3; \]
\[ \text{for } a \geq 3, \]

where

\[ C_7 (k_{\text{min}}, k_{\text{max}}) = \]

\[ \begin{cases} 
\sum I C_8 (I) C_{10} (I), 
\end{cases} \]
\[ \text{for } k_{\text{max}} - k_{\text{min}} = 1 \]
\[ = \begin{cases} 
\sum I_1 \sum I_2 C_8 (I_1) C_9 (I_1, I_2, k_{\text{min}} + 1) C_{10} (I_2), 
\end{cases} \]
\[ \text{for } k_{\text{max}} - k_{\text{min}} = 2 \]
\[ \sum I_1 \sum I_2 C_8 (I_1) C_{11} (I_1, I_2) C_{10} (I_2), \]
\[ \text{for } k_{\text{max}} - k_{\text{min}} < 2 \]
From (8) we have that in the expressions (27), (30), (31) and (32) the ranks \( k \) have no analogue in Cowan (1981).

Expression (33) have also no analogue in Cowan (1981).

Thus, we have studied all possible cases of matrix elements of arbitrary two-electron operators. The expressions for recoupling matrices ((22), (26) and (33)) obtained in this section are simpler and, thus, more convenient for practical applications, than those of Cowan (1981), except for the simplest case \( k = 0 \) of an operator acting on one shell (18), where they are equivalent.
5 Calculation of tensorial quantities

In this section we will consider the submatrix elements

\[ T (n_1 \lambda_1, n_2 \lambda_2, n'_1 \lambda'_1, n'_2 \lambda'_2, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma) \]

appearing in (11). Taking into account, that operators \( a_{m_\lambda}^{(\lambda)} \) and \( \tilde{a}_{m_\lambda}^{(\lambda)} \) are components of the tensor \( a_{m_\lambda}^{(q\lambda)} \), having in quasispin space the rank \( q = \frac{1}{2} \) and projections \( m_q = \pm \frac{1}{2} \), i.e. \( a_{ \frac{1}{2} m_\lambda}^{(q\lambda)} = a_{m_\lambda m_\lambda}^{(qs)} \) and \( a_{ -\frac{1}{2} m_\lambda}^{(q\lambda)} = \tilde{a}_{m_\lambda m_\lambda}^{(ls)} \)
the operators \( A^{(kk')} (n \lambda, \Xi) \), \( B^{(kk')} (n \lambda, \Xi) \), \( C^{(kk')} (n \lambda, \Xi) \), \( D^{(kk')} (n \lambda, \Xi) \) (see (5)-(8)) in our case correspond, respectively, to the following five expressions:

\[
a^{(q_1 q_2)}_{m_\lambda m_\lambda} \left[ a^{(q)}_{m_\lambda} \times a^{(q)}_{m_\lambda} \right]^{(\sigma_1 \sigma_2)}, \quad (34)
\]

\[
\left[ a^{(q_1 q_2)}_{m_\lambda m_\lambda} \times a^{(q_3 q_4)}_{m_\lambda m_\lambda} \right]^{(\sigma_1 \sigma_2)}, \quad (35)
\]

\[
\left[ a^{(q_1 q_2)}_{m_\lambda m_\lambda} \times a^{(q_3 q_4)}_{m_\lambda m_\lambda} \right]^{(\sigma_1 \sigma_2)}, \quad (36)
\]

\[
\left[ a^{(q_1 q_2)}_{m_\lambda m_\lambda} \times a^{(q_3 q_4)}_{m_\lambda m_\lambda} \right]^{(\sigma_1 \sigma_2)}, \quad (37)
\]

\[
\left[ a^{(q_1 q_2)}_{m_\lambda m_\lambda} \times a^{(q_3 q_4)}_{m_\lambda m_\lambda} \right]^{(\sigma_1 \sigma_2)}, \quad (38)
\]

We will discuss the derivation of submatrix elements of these operators, and present the expressions for these quantities. It is worth noting that these tensorial quantities all act upon the same shell. So, all the advantages of tensor algebra and the quasispin formalism may be exploited efficiently.

We obtain the submatrix elements of operator (34) by straightforwardly using the Wigner-Eckart theorem in quasispin space:

\[
\left( l^N a^{(q_1 q_2)}_{m_\lambda m_\lambda} \right) (l^{k\prime} \alpha' Q'L'S') = - |Q|^{-1/2} \left[ Q' M'_Q \right]^{1/2} \times \left( l a^{(q_1 q_2)}_{m_\lambda m_\lambda} Q M_Q \right)
\]

where the last multiplier in (39) is the so-called completely reduced (reduced in the quasispin, orbital and spin spaces) matrix element. The coefficient

\[
\left[ \begin{array}{ccc} j_1 & j_2 & j \\ m_1 & m_2 & m \end{array} \right]
\]

is a Clebsch-Gordan coefficient. Different notations for it occur, e.g. \( A^{j_1 j_2}_{m_1 m_2} \) in Eckart (1930), \( S^{j_1 j_2}_{m_1 m_2} \) in Wigner (1931), \( h_{j_1 m_1 m_2 j_2 m_2} \) in Condon and Shortley (1935) or Judd (1967).

The value of the submatrix element of operator (35) is obtained by basing our development on (33), (34) of Gaigalas and Rudzikas (1996). In the other three cases (36), (37), (38) we obtain them by using (2.28) of
Jucys and Savukynas (1973):

$$\langle nl^N \alpha QLS || F^{(k_1 \sigma_1)}(n\lambda) \times G^{(k_2 \sigma_2)}(n\lambda) \rangle^{(kk)} || nl^{N'} \alpha' Q'L'S' \rangle =$$

$$=(-1)^{L+S+L'+S'+2k}[k] \times$$

$$\sum_{\alpha''} \langle nl^N \alpha QLS || F^{(k_1 \sigma_1)}(n\lambda) || nl^{N''} \alpha'' Q'' L'' S'' \rangle \times$$

$$\langle nl^{N''} \alpha'' Q'' L'' S'' || G^{(k_2 \sigma_2)}(n\lambda) || nl^{N'} \alpha' Q'L'S' \rangle \times$$

$$\left\{ \begin{array}{c} \kappa_1 \\ \kappa_2 \\ k \end{array} \right\} \left\{ \begin{array}{c} \sigma_1 \\ \sigma_2 \\ k \end{array} \right\} \left\{ \begin{array}{c} L' \\ L \\ L'' \end{array} \right\} \left\{ \begin{array}{c} S' \\ S \\ S'' \end{array} \right\},$$

(40)

where $F^{(k_1 \sigma_1)}(n\lambda)$, $G^{(k_2 \sigma_2)}(n\lambda)$ is one of (34) or (35) and the submatrix elements correspondingly are defined by (39) and (33), (34) of Gaigalas and Rudzikas (1996). $N''$ is defined by the second quantization operators occurring in $F^{(k_1 \sigma_1)}(n\lambda)$ and $G^{(k_2 \sigma_2)}(n\lambda)$.

As is seen, by using this approach, the calculation of the angular parts of matrix elements between functions with $u$ open shells is reduced to requiring the submatrix elements of tensors (34) and (35) within one shell of equivalent electrons. As these completely reduced submatrix elements do not depend on the occupation number of the shell, the tables for these quantities are considerably reduced in size in comparison with the tables of analogous submatrix elements of tensorial quantities $U^k$, $V^{k_1 k_2}$ (Jucys and Savukynas 1973) and the tables of fractional parentage coefficients.

### 6 Phase factor

In this section we present the phase factors $\Delta$ in (11), which appear for submatrix elements of operators in Eq. (5)-(8).

For distributions 1-6 (Table 1):

$$\Delta = 0.$$  \hspace{1cm} (41)

For the distributions 7-18 (Table 1):

$$\Delta = 1 + \sum_{k=i}^{i-1} N_k,$$  \hspace{1cm} (42)

where if $\alpha < \beta$, then $i = \alpha$, $j = \beta$, and if $\alpha > \beta$, then $i = \beta$, $j = \alpha$; $N_k$ is the occupation number of a shell of equivalent electrons having the label $k$. For the distributions 19-42 (Table 1):

$$\Delta = \sum_{k=\alpha}^{\beta-1} N_k + \sum_{k=\gamma}^{\delta-1} N_k.$$  \hspace{1cm} (43)

### 7 Spin-angular part of any two-particle operator
Table 8: Scheme of the expressions for matrix elements of any two-particle operator

| No. | $\hat{G}$ | $\hat{G}(T)$ | $\alpha$ | $\beta$ | $\gamma$ | $\delta$ | $\hat{\Theta}$ | $R$ | $\Delta$ |
|-----|----------|-------------|---------|--------|---------|--------|-------------|-----|--------|
| 1.  | (44)     | (5)         | (38)    | –      | –       | –      | (45)        | (14), (18) | (41)   |
|     | (47)     | (5)         | (38)    | –      | –       | –      | (48), (49)  | (14), (18) | (41)   |
| 2.  | (50)     | (6)         | (35)    | (35)   | –       | –      | (51)        | (19), (22) | (41)   |
| 3.  | (50)     | (6)         | (35)    | (35)   | –       | –      | (51)        | (19), (22) | (41)   |
| 4.  | (54)     | (6)         | (35)    | (35)   | –       | –      | (55)        | (19), (22) | (41)   |
| 5.  | (54)     | (6)         | (35)    | (35)   | –       | –      | (55)        | (19), (22) | (41)   |
| 6.  | (52)     | (6)         | (35)    | (35)   | –       | –      | (53)        | (19), (22) | (41)   |
| 7.  | (56)     | (6)         | (36)    | (34)   | –       | –      | (58)        | (19), (22) | (42)   |
| 8.  | (56)     | (6)         | (36)    | (34)   | –       | –      | (59)        | (19), (22) | (42)   |
| 9.  | (60)     | (6)         | (34)    | (37)   | –       | –      | (62)        | (19), (22) | (42)   |
| 10. | (60)     | (6)         | (34)    | (37)   | –       | –      | (63)        | (19), (22) | (42)   |
| 11. | (50)     | (7)         | (34)    | (34)   | (35)    | –      | (51)        | (24), (26) | (42)   |
| 12. | (50)     | (7)         | (34)    | (34)   | (35)    | –      | (51)        | (24), (26) | (42)   |
| 13. | (54)     | (7)         | (34)    | (34)   | (35)    | –      | (55)        | (24), (26) | (42)   |
| 14. | (54)     | (7)         | (34)    | (34)   | (35)    | –      | (55)        | (24), (26) | (42)   |
| 15. | (52)     | (7)         | (34)    | (34)   | (35)    | –      | (53)        | (24), (26) | (42)   |
| 16. | (52)     | (7)         | (34)    | (34)   | (35)    | –      | (53)        | (24), (26) | (42)   |
| 17. | (52)     | (7)         | (34)    | (34)   | (35)    | –      | (53)        | (24), (26) | (42)   |
| 18. | (52)     | (7)         | (34)    | (34)   | (35)    | –      | (53)        | (24), (26) | (42)   |
| 19. | (52)     | (8)         | (34)    | (34)   | (34)    | (34)   | (53)        | (27), (33) | (43)   |
| 20. | (52)     | (8)         | (34)    | (34)   | (34)    | (34)   | (53)        | (27), (33) | (43)   |
| 21. | (52)     | (8)         | (34)    | (34)   | (34)    | (34)   | (53)        | (27), (33) | (43)   |
| 22. | (52)     | (8)         | (34)    | (34)   | (34)    | (34)   | (53)        | (27), (33) | (43)   |
In the previous sections, all the expressions required to calculate the spin-angular part of any two-particle operator were given. For convenience, the structure of the expressions (the numbers of the corresponding formulas) are summarized in the Table 8 for each distribution given in the Table 1. The classification numbers of the distributions are presented in the first column of the Table 8. The equation number of the tensorial expression of the two-particle operator $\hat{G}$ is given in the second column, and the equation number of the tensorial class of the two-particle operator, denoted by $\hat{G}(T)$, in the third column. In the next four columns are given the numbers of the formulas of the tensors, which act inside the shell. A tensor acting upon the $\alpha$ shell is given in the $\alpha$ column, and in the columns $\beta$, $\gamma$, $\delta$ - upon the $\beta$, $\gamma$, $\delta$ shells, respectively. Consequently, if we want to find submatrix element, $T \left( n_i \lambda_i, n_j \lambda_j, n'_i \lambda'_i, n'_j \lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma \right)$, at first we have to calculate the submatrix element of the tensor from column $\alpha$ between functions, consisting only of the $\alpha$ shell, and then to look for the submatrix element of the tensor from column $\beta$ between functions, consisting only of $\beta$ shell, and so on. Thus, we need to calculate only submatrix elements of the tensors acting upon a certain shell. The details of the calculation of these submatrix elements were discussed in the Section 5.

The coefficients $\hat{\Theta}$ are given in the $\hat{\Theta}$ column. The numbers of expressions for the recoupling matrix $R \left( \lambda_i, \lambda_j, \lambda'_i, \lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma \right)$ and phase factor $\Delta$ are given in the last two columns. From this table it is easy to derive the general formulas for spin-angular parts of matrix elements of any two-particle operator.

### Table 8 (continued)

| No. | $\hat{G}$ | $\hat{G}(T)$ | $\alpha$ | $\beta$ | $\gamma$ | $\delta$ | $\hat{\Theta}$ | $R$ | $\Delta$ |
|-----|--------|-------------|---------|---------|---------|---------|--------------|-----|--------|
| 23. | (52)   | (8)         | (34)    | (34)    | (34)    | (34)    | (53)         | (27), (33) | (43)   |
| 24. | (52)   | (8)         | (34)    | (34)    | (34)    | (34)    | (53)         | (27), (33) | (43)   |
| 25. | (52)   | (8)         | (34)    | (34)    | (34)    | (34)    | (53)         | (27), (33) | (43)   |
| 26. | (52)   | (8)         | (34)    | (34)    | (34)    | (34)    | (53)         | (27), (33) | (43)   |
| 27. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 28. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
| 29. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 30. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
| 31. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 32. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 33. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
| 34. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
| 35. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 36. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 37. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
| 38. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
| 39. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 40. | (50)   | (8)         | (34)    | (34)    | (34)    | (34)    | (51)         | (27), (33) | (43)   |
| 41. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
| 42. | (54)   | (8)         | (34)    | (34)    | (34)    | (34)    | (55)         | (27), (33) | (43)   |
8 Conclusions

The approach to matrix element evaluation that we present, is based on the combination of the angular momentum theory as described in Jucys and Bandzaitis (1977), on the concept of irreducible tensorial sets (Judd 1967, Rudzikas and Kaniauskas 1984), on a generalized graphical approach (Gaigalas et al 1985), on the quasispin approach (Rudzikas and Kaniauskas 1984), and on the use of reduced coefficients of fractional parentage (Rudzikas 1991, Rudzikas 1997, Judd 1996). All this, in its entity, introduces a number of new features, in comparison with traditional approaches:

(1) The tensorial expressions of a two-particle operator, presented in Section 2, allow one to exploit all the advantages of a new version of Racah algebra based on quasispin formalism when the latter is applied within each particular shell only. In particular, this is not only a reformulation of spin-angular calculations in terms of standard quantities, but also the determination beforehand from symmetry properties, of which matrix elements are equal to zero without performing further explicit calculations. That is determined from the submatrix elements $T(n_i\lambda_i, n_j\lambda_j, n_i'\lambda'_i, n_j'\lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)$.

(2) It enables one to use the Wigner-Eckart theorem in quasispin space. This provides an opportunity to use tables of reduced coefficients of fractional parentage and tables of other standard quantities (Section 5), which do not depend on the occupation number of a shell of equivalent electrons. Thus, the volume of tables of standard quantities is reduced considerably in comparison with the analogous tables of submatrix elements of tensorial operators $U^k, V^{k1}$ and the tables of fractional parentage coefficients. This undoubtedly makes the inclusion of shells of equivalent $f$ electrons with arbitrary occupation numbers considerably easier, and the process of selecting the standard quantities from the tables becomes simpler.

(3) The tensorial form of any operator presented in Section 2 allows one to obtain simple expressions for the recoupling matrices (Section 4). Hence, the computer code based on this approach would use immediately the analytical formulas for recoupling matrices $R(\lambda_i, \lambda_j, \lambda'_i, \lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Gamma)$. This feature also saves computing time, because i) complex calculations leading finally to simple analytical expressions (Bar-Shalom and Klapisch 1988) are avoided, and ii) a number of momenta triads (triangular conditions) can be checked before the explicit calculation of a recoupling matrix leading to a zero value. These triangular conditions may be determined not only for the terms of shells that the operators of second quantization act upon, as is the case for the submatrix elements $T(n_i\lambda_i, n_j\lambda_j, n_i'\lambda'_i, n_j'\lambda'_j, \Lambda^{bra}, \Lambda^{ket}, \Xi, \Gamma)$ (see conclusion 1), but also for the rest of the shells and resulting terms.

In this approach both diagonal and non-diagonal with respect to configurations, matrix elements are considered in a uniform way, and are expressed in terms of the same quantities. The difference is only in the values of the projections of the quasispin momenta of separate shells.

In this paper all the expressions needed in the spin-angular parts of matrix elements of two-particle operators calculation are presented. This approach is applicable to one-particle operators as well. While calculating the spin-angular parts of the latter, all the expressions needed are included in the cases discussed for the two-particle operator. For instance, in the recoupling matrix calculation two of the four cases discussed above appear, namely, when all the second quantization operators act upon the same shell (Section 4.1) and when they act upon two different shells of equivalent electrons (Section 4.2). Thus, this approach is applicable to any one- and two-particle operator. Practical usage shows that a series of difficulties persisting in the traditional approach to the calculation of angular parts of matrix elements based on the usage of coefficients of fractional parentage and unit tensors can be avoided and high efficiency may be achieved. Indeed, preliminary calculations show that computer programs based on our approach on average are 4-6 times faster than the other well-known codes (Gaigalas et al 1995). This methodology can easily be generalized to cover the case of relativistic operators and relativistic wave functions.
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Appendix

Here algebraic expressions are presented for the two-particle operator (1) in the irreducible tensorial form for all the distributions from Table 8. Although there are quite a few distributions, the structure of their algebraic formulas is similar, and therefore on the basis of a graphical approach (Gaigalas et al 1985) the expressions may be written down in a compact form, where one general formula includes all the cases having the same structure. Each particular formula is obtained from these by performing elementary graphical transformations according to the rules explained below. The general expressions are:

(1) Distribution αααα (case 1 from Table 8):

For this distribution the analytical expressions (7), (8) in Gaigalas and Rudzikas (1996) are used, in which the quantum numbers \( n_i l_i, n_j l_j, n_i' l_i', n_j' l_j' \) acquire particular values of a shell \( \alpha \). For the first form (Figure 1, \( A_1 \)), we have

\[
A_1 = \sum_{\kappa_1 \sigma_1 \kappa_2 \sigma_2} \tilde{\Theta}_I (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi) \times
\]

\[
\times \left[ a(l_s, s) \times a(l_s, s) \right]^{(\kappa_1 \sigma_1 \kappa_2 \sigma_2)} \times \left[ a'(l_s, s) \times a'(l_s, s) \right]^{(\kappa_1 \sigma_1 \kappa_2 \sigma_2)} \times (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi) \equiv \Theta (n_\alpha \lambda_\alpha, \Xi)
\]

and

\[
\tilde{\Theta}_I (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi) \equiv \Theta' (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi) \equiv \Theta (n_\alpha \lambda_\alpha, \Xi)
\]

In an equivalent second form (Figure 1, \( A_2 + A_3 \)), we have

\[
A_2 + A_3 = \tilde{\Theta}_{Ia} (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi) \times
\]

\[
\times \left[ a(l_s, s) \times a'(l_s, s) \right]^{(\kappa_1 \sigma_1 \kappa_2 \sigma_2)} \times \left[ a'(l_s, s) \times a(l_s, s) \right]^{(\kappa_1 \sigma_1 \kappa_2 \sigma_2)} \times (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi) \equiv \Theta (n_\alpha \lambda_\alpha, \Xi)
\]

\[
\tilde{\Theta}_{Ia} (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi) = \frac{1}{2} (-1)^{k-p} [\kappa_1, \sigma_1, \kappa_2, \sigma_2]^{-1/2} \times
\]

\[
\times (n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, n_\alpha \lambda_\alpha, \Xi)
\]
Figure 1: Diagrams for an arbitrary two-particle operator. Diagrams $A_1$, $A_2$ and $A_3$ represent two-particle operators when this operator has distribution $\alpha\alpha\alpha\alpha$. Diagrams $A_4$ and $A_5$ represent two-particle operators for all others distributions. Diagrams $A_1$, $A_2$, $A_3$, $A_4$ and $A_5$ are similar to the usual Feynman-Goldstone diagrams. Diagrams $A_6$, $A_7$ and $A_8$ represent tensorial products of second quantization operators ($A_6$ for the second group, $A_7$ for the third, and $A_8$ for the fourth.).
and

\[
\tilde{\Theta}_{IIb} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) = (-1)^{k-2+p+1} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) \times \times \left\{ \frac{\kappa_1}{\lambda_1} \frac{\kappa_2}{\lambda_2} \frac{k}{\lambda_3} \left[ \begin{array}{ccc} \sigma_1 & \sigma_2 & k \\ s & s & s \end{array} \right] \right\},
\]

Both factors \(\tilde{\Theta}_{IIa} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi)\) and \(\tilde{\Theta}_{IIb} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi)\) have properties analogous to those of \(\tilde{\Theta}_{I}\) as stated in (45).

(2) Distributions \(\alpha \beta \alpha \beta, \beta \alpha \beta \alpha, \beta \gamma \alpha \gamma, \beta \gamma \alpha \beta, \beta \gamma \beta \alpha, \beta \gamma \beta \alpha\) (cases 2, 3, 11, 12, 27, 29, 31, 32, 35, 36, 39, 40 from Table 8) (Figure 1, A4, A6):

\[
A_4 = \tilde{\Theta} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) A_6, \tag{50}
\]

where

\[
\tilde{\Theta} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) = \frac{1}{2} (-1)^{k-2+p+1} \times \left\{ \begin{array}{ccc} \kappa_1 & \kappa_2 & k \\ \lambda_1 & \lambda_2 & \lambda_3 \end{array} \right\} \times \left\{ \begin{array}{ccc} \sigma_1 & \sigma_2 & k \\ s & s & s \end{array} \right\}.
\]

Diagram \(A_6\) corresponds to tensorial products of the operators of second quantization for two-particle operator (for details see in Gaigalas and Rudzikas 1996).

(3) Distributions \(\alpha \alpha \beta \alpha, \beta \gamma \beta \alpha, \beta \gamma \alpha \beta, \beta \gamma \alpha \beta, \beta \alpha \beta \gamma, \beta \alpha \beta \gamma\) (cases 6, 15-26 from Table 8) (Figure 1, A5, A7):

\[
A_5 = \sum_{\kappa_1 \sigma_1 \kappa_1 \sigma_1} \tilde{\Theta} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) A_7, \tag{52}
\]

where

\[
\tilde{\Theta} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) = \frac{1}{2} (-1)^{k-2+p+1} \times [\kappa_1 \sigma_1, \kappa_2 \sigma_1]^{1/2} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) \times \left\{ \begin{array}{ccc} \kappa_1 & \kappa_2 & k \\ \lambda_1 & \lambda_2 & \lambda_3 \end{array} \right\} \times \left\{ \begin{array}{ccc} \sigma_1 & \sigma_2 & k \\ s & s & s \end{array} \right\}.
\]

(4) Distributions \(\alpha \beta \alpha \beta, \beta \alpha \beta \alpha, \beta \gamma \alpha \gamma, \alpha \beta \gamma \delta, \beta \alpha \gamma \delta, \beta \alpha \gamma \delta, \beta \alpha \gamma \delta, \beta \gamma \alpha \delta, \beta \gamma \alpha \delta\) (cases 4, 5, 13, 14, 28, 30, 33, 34, 37, 38, 41, 42 from Table 8) (Figure 1, A1, A6):

\[
A_1 = \sum_{\kappa_1 \sigma_1 \kappa_1 \sigma_1} \tilde{\Theta} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) A_6, \tag{54}
\]

where

\[
\tilde{\Theta} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) = \frac{1}{2} (-1)^{k-2+p+1+\ell_1^{+}+\ell_2^{+}+\sigma_2+\kappa_1^{+}+\kappa_2^{+}} [\kappa_1 \sigma_1, \kappa_2 \sigma_1]^{1/2} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) \times \left\{ \begin{array}{ccc} \kappa_1 & \kappa_2 & k \\ \lambda_1 & \lambda_2 & \lambda_3 \end{array} \right\} \times \left\{ \begin{array}{ccc} \sigma_1 & \sigma_2 & k \\ s & s & s \end{array} \right\}.
\]

(5) Distributions \(\beta \alpha \alpha \alpha, \alpha \beta \alpha \alpha\) (cases 7, 8 from Table 8) (Figure 1, A5):

\[
A_5 = \sum_{\kappa_1 \sigma_1 \kappa_1 \sigma_1} \tilde{\Theta} (n, \lambda_1, n, \lambda_2, n, \lambda_3, \Xi) \times \left[ a^{(l_1^{+})} \times a^{(l_2^{+})} \times \tilde{a}^{(l_3^{+})} \times \tilde{a}^{(l_4^{+})} \right]^{(k)}_{(l)}, \tag{56}
\]
where
\[ \tilde{\Theta}\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) \equiv \Theta'\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) \equiv \Theta\left(n_\alpha\lambda_\alpha, n_\beta\lambda_\beta, \Xi\right). \] (57)

When \(\tilde{G}(T) = \tilde{G}(\beta\alpha\alpha\alpha)\), then
\[ \tilde{\Theta}\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) = \frac{1}{2} (-1)^{k+p+k_12+\sigma_112+l_\alpha+l_\beta} \left[ k_12, \sigma_112 \right] \times [k_12', \sigma_112']^{1/2} \left[ \left( n_\alpha\lambda_\alpha, n_\beta\lambda_\beta \right)|g_{\alpha\beta}(\kappa_1\kappa_2, \sigma_1\sigma_2)| \right] \left[ n_\alpha\lambda_\alpha, n_\alpha\lambda_\alpha \right] \times \left\{ \begin{array}{ccc} l_\alpha & l_\alpha & \kappa_12 \\ \kappa_1 & \kappa_2 & k \\ l_\beta & l_\beta & \kappa_12 \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_112 \\ \sigma_1 & \sigma_2 & k \\ s & s & \sigma_112 \end{array} \right\} \times \sum_{K_iK_s} [K_i, K_s]^{1/2} \left\{ \begin{array}{ccc} l_\beta & l_\alpha & \kappa_12 \\ \kappa_12' & k & K_i \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_112 \\ \sigma_112 & k & K_s \end{array} \right\}. \] (58)

and when \(\tilde{G}(T) = \tilde{G}(\alpha\beta\alpha\alpha)\), then
\[ \tilde{\Theta}\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) = \frac{1}{2} (-1)^{k+p+k_12+\sigma_112+\sigma_212} \left[ k_12, \sigma_212 \right] \times [k_12', \sigma_212']^{1/2} \left[ \left( n_\alpha\lambda_\alpha, n_\beta\lambda_\beta \right)|g_{\alpha\beta}(\kappa_1\kappa_2, \sigma_1\sigma_2)| \right] \left[ n_\alpha\lambda_\alpha, n_\alpha\lambda_\alpha \right] \times \left\{ \begin{array}{ccc} l_\alpha & l_\alpha & \kappa_12 \\ \kappa_1 & \kappa_2 & k \\ l_\beta & l_\beta & \kappa_12 \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_112 \\ \sigma_1 & \sigma_2 & k \\ s & s & \sigma_112 \end{array} \right\} \times \sum_{K_iK_s} [K_i, K_s]^{1/2} \left\{ \begin{array}{ccc} l_\beta & l_\alpha & \kappa_12 \\ \kappa_12' & k & K_i \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_112 \\ \sigma_112 & k & K_s \end{array} \right\}. \] (59)

(6) Distributions \(\beta\beta\alpha\), \(\beta\alpha\beta\) (cases 9, 10 from Table 8) (Figure 1, A5):
\[ A_5 = \sum_{\kappa_12^{1/2}k_12^{1/2}} \tilde{\Theta}\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) \times \left[ \left[ q_1^{(l_\beta s)} \times q_2^{(l_\beta s)} \right]^{(k_12, \sigma_112)} \tilde{q}_2^{(l_\beta s)} \right]^{(k_12, \sigma_112)} \times \tilde{q}_1^{(l_\alpha s)} \right]_{p,-p}, \] (60)
where
\[ \tilde{\Theta}\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) \equiv \Theta'\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) \equiv \Theta\left(n_\alpha\lambda_\alpha, n_\beta\lambda_\beta, \Xi\right). \] (61)

When \(\tilde{G}(T) = \tilde{G}(\beta\beta\alpha)\):
\[ \tilde{\Theta}\left(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi\right) = \frac{1}{2} (-1)^{k+p+k_12+\sigma_112+l_\alpha+l_\beta} \left[ k_12', \sigma_112 \right] \times [k_12, \sigma_112']^{1/2} \left[ \left( n_\beta\lambda_\beta, n_\beta\lambda_\beta \right)|g_{\beta\beta}(\kappa_1\kappa_2, \sigma_1\sigma_2)| \right] \left[ n_\beta\lambda_\beta, n_\alpha\lambda_\alpha \right] \times \left\{ \begin{array}{ccc} l_\beta & l_\alpha & \kappa_12 \\ \kappa_1 & \kappa_2 & k \\ l_\beta & l_\beta & \kappa_12 \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_112 \\ \sigma_1 & \sigma_2 & k \\ s & s & \sigma_112 \end{array} \right\} \times \sum_{K_iK_s} [K_i, K_s]^{1/2} \left\{ \begin{array}{ccc} l_\alpha & l_\beta & \kappa_12 \\ \kappa_12' & k & K_i \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_112 \\ \sigma_112 & k & K_s \end{array} \right\}. \] (62)
and when $\hat{G}(T) = \hat{G}(\beta\beta\alpha\beta)$:

$$\tilde{\Theta}(n_i\lambda_i, n_j\lambda_j, n_i'\lambda_i', n_j'\lambda_j', \Xi) = \frac{1}{2} (-1)^{k - p + \kappa_1' + \sigma_1' + \kappa_1 + \sigma_1} [\kappa_1', \sigma_1', \kappa_1, \sigma_1] \times$$

$$\times [\kappa_1, \sigma_1]^{1/2} \langle n_\beta n_\gamma | g^{(\kappa_1\kappa_2\kappa_3\kappa_4)\sigma_1\sigma_2\sigma_3\sigma_4} | n_\alpha n_\lambda \rangle \times$$

$$\times \left\{ \begin{array}{ccc} l_\alpha & l_\beta & \kappa_1 \\ \kappa_1 & \kappa_2 & k \\
\end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_1 \\ \kappa_1 & \kappa_2 & k \\
\end{array} \right\} \times$$

$$\times \sum_{K_i K_s} [K_i, K_s]^{1/2} \left\{ \begin{array}{ccc} l_\alpha & l_\beta & \kappa_1' \\ \kappa_1' & \kappa_2 & k \\
\end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_1' \\ \kappa_1' & \kappa_2 & k \\
\end{array} \right\} . \quad (63)$$

The final analytical expressions for diagram $A_5$ appearing in (50), diagram $A_7$ in (52) and diagram $A_8$ in (54), are obtained after the following graphical transformations:

(i) The second quantization operators are interchanged, until (from left to right) first come the operators acting upon shell $\alpha$, then correspondingly upon $\beta$, $\gamma$, $\delta$.

(ii) The generalized Clebsch-Gordan coefficient is transformed to match the order of operators. This is performed by changing the order of angular momenta coupling at some of the nodes 1, 2, 3 (Figure 1, $A_6$, $A_7$ and $A_8$).

We write down immediately the algebraic expressions for diagrams $A_6$, $A_7$ and $A_8$ (of Figure 1) after transformation (i) and (ii) by applying usual generalized graphical technique (see Gaigalas et al 1985). Also we have to notice that $\Theta'$ is equal to $\tilde{\Theta}$ with a phase factor, which is found by transforming the diagram of the tensorial structure according to the rules (i) and (ii). Only in cases 1 and 7-10 (see Table 8) is $\Theta' \equiv \tilde{\Theta}$, because there is no need to transform the tensorial structure.

* * *

As an example, let us consider in particular the case where operator $a_j$ acts upon the first shell $n_1\lambda_1$, operator $a_i$ acts upon the second shell $n_2\lambda_2$, and operators $a_i^\dagger$, $a_j^\dagger$, act upon the third shell $n_3\lambda_3$ (see Eq. (1)). This is the distribution 18 in Table 8. We obtain the algebraic expression for distribution $\beta\alpha\gamma\gamma$ from (52). The two-particle operator for this distribution can be represented by diagram $B_1$ which is proportional to its tensorial part (diagram $B_2$) as (Figure 2 $B_1$, $B_2$):

$$B_1 = \sum_{\kappa_{12}\sigma_{12} \kappa_{12}' \sigma_{12}'} \tilde{\Theta}(n_\lambda_2, n_\lambda_1, n_\lambda_3, n_\lambda_3, \Xi) B_2, \quad (64)$$

where

$$\tilde{\Theta}(n_\lambda_2, n_\lambda_1, n_\lambda_3, n_\lambda_3, \Xi) = \frac{1}{2} (-1)^{k - p + 1} [\kappa_{12}, \sigma_{12}, \kappa_{12}', \sigma_{12}']^{1/2} \times$$

$$\times (n_\lambda_2 n_\lambda_1 | g^{(\kappa_{12}\kappa_{12}'\kappa_1\kappa_2\kappa_3\kappa_4\sigma_1\sigma_2\sigma_3\sigma_4)} | n_\lambda_3 n_\lambda_3) \times$$

$$\times \left\{ \begin{array}{ccc} l_2 & l_3 & \kappa_1 \\ \kappa_1 & \kappa_2 & k \\
\end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_1 \\ \kappa_1 & \kappa_2 & k \\
\end{array} \right\} . \quad (65)$$

We use (i) for diagram $B_2$ (Figure 2, $B_2$) then. As in the expression (64) the order of second quantization operators is $a(l_2) a(l_1) a(l_3) a(l_3)^\dagger$, so we change it according to (i) and obtain (Figure 2 $B_1$, $B_3$):

$$B_1 = - \sum_{\kappa_{12} \sigma_{12} \kappa_{12}' \sigma_{12}'} \tilde{\Theta}(n_\lambda_2, n_\lambda_1, n_\lambda_3, n_\lambda_3, \Xi) B_3. \quad (66)$$

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Figure 2: Diagrams for distribution $a^{(l_2s)}a^{(l_1s)}\bar{a}^{(l_3s)}\bar{a}^{(l_3s)}$. Diagram $B_1$ represents a two-particle operator $\hat{G}$. Diagrams $B_2$, $B_3$ and $B_4$ represent graphical transformations. Diagram $B_2$ represents the tensorial part of the two-particle operator $B_1$ before transformations, diagram $B_3$ represents this tensorial part after transformation i), and diagram $B_4$ represents it after transformation ii).
We use (ii) for diagram $B_3$ then. We change the sign at the node 1 to obtain finally (Figure 2 $B_1$, $B_4$):

$$B_1 = \sum_{\kappa_{12}\sigma_{12}\kappa'_{12}\sigma'_{12}} (-1)^{l_{1}+l_{2}+2s-\kappa_{12}-\sigma_{12}+1} \times \Theta(n_{2}\lambda_{2}, n_{1}\lambda_{1}, n_{3}\lambda_{3}, n_{3}\lambda_{3}, \Xi) B_4 =$$

$$= \sum_{\kappa_{12}\sigma_{12}\kappa'_{12}\sigma'_{12}} \Theta'(n_{2}\lambda_{2}, n_{1}\lambda_{1}, n_{3}\lambda_{3}, n_{3}\lambda_{3}, \Xi) B_4 =$$

$$= \sum_{\kappa_{12}\sigma_{12}\kappa'_{12}\sigma'_{12}} \Theta'(n_{2}\lambda_{2}, n_{1}\lambda_{1}, n_{3}\lambda_{3}, n_{3}\lambda_{3}, \Xi) \times$$

$$\times \left[ a(l_{1}s) \times a(l_{2}s) \right]^{(\kappa_{12}\sigma_{12})} \times \left[ \bar{a}(l_{3}s) \times \bar{a}(l_{3}s) \right]^{(\kappa'_{12}\sigma'_{12})}_{p,-p},$$

(67)

where

$$\Theta'(n_{2}\lambda_{2}, n_{1}\lambda_{1}, n_{3}\lambda_{3}, n_{3}\lambda_{3}, \Xi) = \Theta(n_{1}\lambda_{1}, n_{2}\lambda_{2}, n_{3}\lambda_{3}, \Xi) =$$

$$= (-1)^{l_{1}+l_{2}+2s-\kappa_{12}-\sigma_{12}+1} \Theta(n_{2}\lambda_{2}, n_{1}\lambda_{1}, n_{3}\lambda_{3}, n_{3}\lambda_{3}, \Xi) =$$

$$= \frac{1}{2} \sum_{\kappa_{12}\sigma_{12}\kappa'_{12}\sigma'_{12}} (-1)^{k-p+l_{1}+l_{2}+2s-\kappa_{12}-\sigma_{12}+1} \left[ \kappa_{12}, \sigma_{12}, \kappa'_{12}, \sigma'_{12} \right]^{1/2} \times$$

$$\times \left( n_{2}\lambda_{2} n_{1}\lambda_{1} \left| g^{(\kappa_{12}\kappa'_{12}, \sigma_{12}\sigma'_{12})} \right| n_{3}\lambda_{3} n_{3}\lambda_{3} \right) \times$$

$$\times \left\{ \begin{array}{ccc} l_{2} & l_{3} & \kappa_{1} \\ l_{1} & l_{3} & \kappa_{2} \\ \kappa_{12} & \kappa'_{12} & k \end{array} \right\} \left\{ \begin{array}{ccc} s & s & \sigma_{1} \\ s & s & \sigma_{2} \\ \sigma_{12} & \sigma'_{12} & k \end{array} \right\}.$$

(68)

All the graphical transformations are made and the correspondence between angular momentum diagrams $B_2$, $B_3$ and $B_4$ in Figure 2 and algebraic expressions is defined according to the graphical approach of Gaigalas et al (1985).

Now using (67) and (68) we can write down the irreducible tensorial form for the Coulomb operator with tensorial structure $\kappa_1 = \kappa_2 = k$, $\sigma_1 = \sigma_2 = 0$, $k = 0$ and the two-electron submatrix element:

$$\left( n_{2}\lambda_{2} n_{1}\lambda_{1} \left| g_{\text{Coulomb}}^{(k,0,0,0)} \right| n_{3}\lambda_{3} n_{3}\lambda_{3} \right) =$$

$$= 2 \left[ k \right]^{1/2} \left( l_{2} \left| C^{(k)} \right| l_{3} \right) \left( l_{1} \left| C^{(k)} \right| l_{3} \right) R_{k} \left( n_{2} l_{2} n_{3} l_{3}, n_{1} l_{1} n_{3} l_{3} \right).$$

(69)

From (68) we have:

$$\left[ \Theta_{\text{Coulomb}}(n_{2}\lambda_{2}, n_{1}\lambda_{1}, n_{3}\lambda_{3}, n_{3}\lambda_{3}, \Xi) = \right.$$

$$\left. = \frac{1}{2} \sum_{\kappa_{12}\sigma_{12}\kappa'_{12}\sigma'_{12}} (-1)^{l_{1}+l_{2}+2s-\kappa_{12}-\sigma_{12}+1} \left[ \kappa_{12}, \sigma_{12}, \kappa'_{12}, \sigma'_{12} \right]^{1/2} \timesight.$$

$$\left. \times 2 \left[ k \right]^{1/2} \left( l_{2} \left| C^{(k)} \right| l_{3} \right) \left( l_{1} \left| C^{(k)} \right| l_{3} \right) R_{k} \left( n_{2} l_{2} n_{3} l_{3}, n_{1} l_{1} n_{3} l_{3} \right) \timesight.$$}

$$\times \left\{ \begin{array}{ccc} l_{2} & l_{3} & k \\ l_{1} & l_{3} & k \\ \kappa_{12} & \kappa'_{12} & 0 \end{array} \right\} \left\{ \begin{array}{ccc} s & s & 0 \\ s & s & 0 \end{array} \right\} =$$

$$= -\frac{1}{2} \sum_{\kappa_{12}\sigma_{12}} (-1)^{l_{1}+l_{3}+2s+k} \left[ \kappa_{12}, \sigma_{12} \right]^{1/2} \times$$

$$\times \left( l_{2} \left| C^{(k)} \right| l_{3} \right) \left( l_{1} \left| C^{(k)} \right| l_{3} \right) R_{k} \left( n_{2} l_{2} n_{3} l_{3}, n_{1} l_{1} n_{3} l_{3} \right) \left\{ \begin{array}{ccc} l_{2} & l_{3} & k \\ l_{3} & l_{1} & \kappa_{12} \end{array} \right\}. \right.$$
This kind of operator needs to be calculated when we are considering, for example, the matrix element 

\[
\langle 3s^23d^2L_1S_1Q_1L_2S_2Q_2LS || H_{\text{Coulomb}} || 3s3d^2p^2L'_1S'_1Q'_1L'_2S'_2Q'_2L''_1S''_1Q''_1L''_2S''_1Q''_2L''_3S''_2Q''_3L''S'' \rangle.
\]

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