Second Quantization and Coefficients of Fractional Parentage

ANDRIUS BERNOTAS AND JULIUS KANIAUSKAS

Institute of Theoretical Physics and Astronomy, A. Goštauto 12, 2600 Vilnius, Lithuania

E-mail: bernotas@itpa.lt

Abstract. The coefficients of fractional parentage (CFPs), treated by tradition as antisymmetrizing multipliers, do not exist as such in the second-quantization representation, because, therein, by definition, there is nothing to antisymmetrize. This by no way means that the above-mentioned representation is less relevant in theoretical atomic spectroscopy than is any other one. On the contrary, all the well-known mathematical apparatus is still successfully applied, alongside with numerous new useful features. Moreover, the analysis presented here yields some results not so obvious from the point of view of the coordinate representation, namely, the consequent application of the second-quantization representation led us to an expansion of many-shell wave functions employing analogs of many-shell CFPs, which appeared to be considerably simpler than the traditional CFPs expansion. Also, a generalization of Redmond's formula for the case of many-shell CFPs and a straightforward method of deriving summation rules for products of CFPs are clear in the second-quantization representation and are sketched here.

‡ INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. 50, 293-315 (1994)

1. Introduction

In second-quantization representation (SQR), the antisymmetry of the wave functions is embedded in the representation itself through the anticommutation properties of single-particle creation and annihilation operators. Since any wave function is antisymmetric, seemingly, there is no sense in antisymmetrizing it with the aid of the coefficients of fractional parentage (CFPs). Here, we remind that the aspect of antisymmetrization is dominant in a common definition of CFPs. While applying SQR, this seeming paradox is solved by realizing that the CFPs, in fact, allow one to form up a basis from a set of linearly dependent wave functions rather than manifest themselves as the antisymmetrizing coefficients. Thus, the interpretation of CFPs, which in second-quantization formalism are represented by the reduced matrix elements of creation operators [1, 2], is completely different in SQR. This difference, however, does not imply any serious changes in the application of the theoretical apparatus developed initially for the coordinate representation (CR). Therefore, SQR, due to pioneer work by Judd [1], became fully applicable [3] alongside with the traditional CR.

A specific gain with the use of SQR, as noted already in [1], is the simple and direct treatment of the properties of configurations that depend on the number of electrons and the transparent application of tensor-operator methods of Racah (see [3] and, e.g., a monograph [4] on isospin and quasispin methods for atoms). Even more, it appears that the consistent application of totally antisymmetric wave functions, or SQR, rather than usage of nonantisymmetric those defined in CR, is of value in dealing with the problem of many-shell CFPs. Also, one of the main points in this article was to prove this.

First, we present the derivation of a new expansion of antisymmetric basis functions that correspond to a fixed general configuration, in a form similar to the CR many-shell CFPs expansion, but simpler. The analogies and differences in CR are traced. Then, we investigate the properties of the new expansion coefficients and show their proportionality to the conventional CFPs. Finally we outline the way to obtain recurrent relationships and product summation rules for the coefficients discussed, presenting some examples. We conclude with brief mention of the utility of the results obtained.

2. Fractional Parentage Expansion in Second-quantization Representation

The known simple mutual correspondence between single-electron orbitals in SQR and CR is sufficient to determine the simple correspondence between orthonormal bases of antisymmetric coupled momenta functions for general multielectron atomic configurations. The first correspondence mentioned we write down as

$$a_{i\,m}^{(\lambda)}\,|0\rangle \Longleftrightarrow \phi(n_i\lambda m)\ , \tag{1}$$

where λ denotes one-electron quantum numbers of angular momentum type: l and s (or j in $j-j$ coupling), and m are their z-projection quantum numbers; it is implied that different notations $a_1, a_2, a_3, \ldots$ correspond to the different shells with their principal quantum numbers being $n_1, n_2, n_3, \ldots$. (It should be stressed that we use notation a rather than $a^\dagger$ for the creation operator, rejecting the popular notation on purpose, following Dirac [5] and reserving the "†" for denoting Hermitian conjugation; since only $\tilde{a}\,{}^{(\lambda)}_{-m} = (-1)^{\lambda+m}\left(a^{(\lambda)}_{m}\right)^\dagger$ but not just $(a^{(\lambda)}_{m})^\dagger$ is a tensor in angular momenta space, with "$\sim$" for annihilation, there should be no confusion between the creation and annihilation tensorial operators.) The simple mutual correspondence between (normalized) SQR and CR determinantal wave functions may be written in the form

$$a_{\beta_N} \ldots a_{\beta_1} |0\rangle \Longleftrightarrow [N!]^{-1/2} \left| \begin{vmatrix} |\phi(\beta_1, x_1)\rangle & \ldots & |\phi(\beta_1, x_N)\rangle \\ \ldots & \ldots & \ldots \\ |\phi(\beta_N, x_1)\rangle & \ldots & |\phi(\beta_N, x_N)\rangle \end{vmatrix} \right\rangle , \tag{2}$$

where quantum numbers β_i (and coordinates x_i) appear in the natural order $\beta_1\beta_2 \ldots \beta_N$, $x_1 x_2 \ldots x_N$. Then,

$$a_{\beta_{N+1}} a_{\beta_N} \ldots a_{\beta_1} |0\rangle \Longleftrightarrow [(N+1)!]^{-1/2} \left| \begin{vmatrix} |\phi(\beta_1, x_1)\rangle & \ldots & |\phi(\beta_1, x_{N+1})\rangle \\ \ldots & \ldots & \ldots \\ |\phi(\beta_{N+1}, x_1)\rangle & \ldots & |\phi(\beta_{N+1}, x_{N+1})\rangle \end{vmatrix} \right\rangle , \tag{3}$$

i.e., not only one more row and column appears in the determinant, but the factor $(N+1)^{-1/2}$ should also be included.

We note that hereafter we will mark the wave functions normalized to unity with a subscript "*N*", the antisymmetric ones with "*A*", and the ones from orthogonal basis with "*O*".

We treat the bases of antisymmetric orthonormal functions for an atomic N-electron system, which are irreducible tensors in certain well-defined angular momentum type spaces, as the linear combinations of the products of single-particle creation operators acting upon the vacuum state (see (2)): $N = N_1 + \ldots + N_k$; k is the number of shells, Λ and M denote the quantum numbers of total angular momentum type and their z-projections, respectively, and α are the additional labels if necessary to distinguish the functions with the same ΛM. The symbol C^Nshould be understood as a compact form of writing down a configuration $n_1\lambda_1^{N_1} \ldots n_i\lambda_k^{N_k}$. Let us take all the kets of such a basis and form up a one-row matrix, its columns labeled by different arrays $\alpha\Lambda M$:

$$\left(\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\,|0\rangle\right)_{row} . \tag{4}$$

The Hermitian conjugate of (4) is a one-column matrix of the corresponding bras:

$$\left(\langle 0|\,\widehat{\Phi}^\dagger_{ONA}(C^N\alpha\Lambda M)\right)_{column} . \tag{5}$$

Then, any antisymmetric ket or bra wave function corresponding to a state of configuration $n_1\lambda_1^{N_1} \ldots n_i\lambda_k^{N_k}$ can be projected with the aid of the operator

$$\widehat{\mathbf{P}} = \left(\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\,|0\rangle\right)_{row} \times \left(\langle 0|\,\widehat{\Phi}^\dagger_{ONA}(C^N\alpha\Lambda M)\right)_{column} \tag{6}$$

onto the basis (4) or (5). The analogs of (4), (5), and (6) are obvious in the CR wave functions basis, where we write $\{_N x\}$ in a CR function for an array of numbered spatial coordinates:

$$\left|\Phi_{ONA}(C^N \alpha \Lambda M\{_N x\})\right\rangle \Longleftrightarrow \widehat{\Phi}_{ONA}(C^N \alpha \Lambda M)\,|0\rangle \ . \tag{7}$$

The basis of uncoupled momenta functions

$$\begin{aligned}
&\left(\left|\Phi_{NA}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row} \\
&= \left([N!]^{-1/2} \left| \begin{vmatrix} |\phi\,(n_1\lambda_1 m_1, x_1)\rangle & \dots & |\phi\,(n_1\lambda_1 m_1, x_N)\rangle \\ \dots & \dots & \dots \\ |\phi\,(n_i\lambda_k m_N, x_1)\rangle & \dots & |\phi\,(n_i\lambda_k m_N, x_N)\rangle \end{vmatrix} \right\rangle \right)_{row} \\
&\Longleftrightarrow \left(a_i{}^{(\lambda_k)}_{m_N} \dots a_1{}^{(\lambda_1)}_{m_1}\,|0\rangle\right)_{row}
\end{aligned} \tag{8}$$

also spans the functional space determined by the basis (7) and can be used to build up the projector. The columns of (8) are labeled by different arrays $\{_N m\}$ (the configuration C^N and ordering in $\{_N x\}$ are fixed). But then, in fact, the space defined by functions (7) is overspanned by the basis (8), because we have linearly dependent functions in (8). Really, we consider *all* the possible orderings in arrays $\{_N m\}$ that are allowed in a particular configuration $C^N \equiv n_1\lambda_1^{N_1} \dots n_i\lambda_k^{N_k}$. It means that the permutations of projections m_i within the shells of equivalent electrons (i.e., with the same $n_i\lambda_j$) are allowed, while they lead only to the change in sign of a wave function at most. Each *essentially different* function now comes $(N_1! \cdot \ldots \cdot N_k!) \equiv \prod N_j!$ times into the one-row matrix (8), the functions therein are not orthogonal, and the basis is an overdetermined one. Thus, we infer that the space of functions (7) is spanned $\prod N_j!$ times by the functions of basis (8). While projecting onto this basis, one should bear that factor in mind:

$$\begin{aligned}
&\left|\Phi_{ONA}(C^N \alpha \Lambda M\{_N x\})\right\rangle = \left(\prod_j N_j!\right)^{-1} \\
&\times \left(\left|\Phi_{NA}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row} \left(\left\langle\Phi_{NA}(C^N\{_N m\}\{_N x\})\right|\right)_{column} \\
&\times \left|\Phi_{ONA}(C^N \alpha \Lambda M\{_N x\})\right\rangle \ .
\end{aligned} \tag{9}$$

Let us now turn our attention to the bases of coupled momenta functions. We note that throughout we intend to use the Clebsch-Gordan rather than Wigner coefficients (indeed, the elements of unitary transformation matrix) for coupling the tensorial quantities. For example,

$$\left[T^{(\Lambda_1)} \times U^{(\Lambda_2)}\right]^{(\Lambda)}_{M} = \sum_{M_1 M_2} T^{(\Lambda_1)}_{M_1} U^{(\Lambda_2)}_{M_2} \begin{bmatrix} \Lambda_1 & \Lambda_2 & \Lambda \\ M_1 & M_2 & M \end{bmatrix} \ . \tag{10}$$

Any basis of totally nonantisymmetric although orthonormal functions of coupled momenta with fixed order of coupling A can be obtained from a basis of uncoupled momenta functions totally nonantisymmetric with respect to the interchange of coordinates $\{_N x\}$:

$$\begin{aligned}
&\left(\left|\Phi_{ON}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row}\\
&\equiv \left(|\phi\left(n_1\lambda_1 m_1, x_1\right)\rangle \times \ldots \times |\phi\left(n_i\lambda_k m_N, x_N\right)\rangle\right)_{row} ,
\end{aligned} \tag{11}$$

with the aid of a unitary transformation $\mathbf{U}$:

$$\begin{aligned}
&\left(\left|\Phi_{ON}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M\{_N x\})\right\rangle\right)_{row}\\
&= \left(\left|\Phi_{ON}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row}(\mathbf{U}) ,
\end{aligned} \tag{12}$$

where $\{\Lambda_a\}$ are the arrays of intermediate momenta in the coupling scheme A and the elements of transformation matrix $(\mathbf{U})$ are the (generalized) Clebsch-Gordan coefficients (see e.g. [6]) of the type

$$\begin{bmatrix} \lambda_1 & \ldots & \lambda_k & \Lambda \\ m_1 & \ldots & m_N & M \end{bmatrix}^{\mathrm{A}}_{\{\Lambda_a\}} .$$

(An example of a generalized Clebsch-Gordan coefficient is

$$\begin{aligned}
&\begin{bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \Lambda \\ m_1 & m_2 & m_3 & M \end{bmatrix}^{(\lambda_1\lambda_2(\Lambda_{12})\lambda_3\Lambda)}_{\Lambda_{12}}\\
&= \sum_{M_{12}} \begin{bmatrix} \lambda_1 & \lambda_2 & \Lambda_{12} \\ m_1 & m_2 & M_{12} \end{bmatrix} \begin{bmatrix} \Lambda_{12} & \lambda_3 & \Lambda \\ M_{12} & m_3 & M \end{bmatrix}\\
&= \begin{bmatrix} \lambda_1 & \lambda_2 & \Lambda_{12} \\ m_1 & m_2 & m_1+m_2 \end{bmatrix} \begin{bmatrix} \Lambda_{12} & \lambda_3 & \Lambda \\ m_1+m_2 & m_3 & M \end{bmatrix} , \text{ of course;}
\end{aligned}$$

an equality

$$\begin{aligned}
&\begin{pmatrix} \langle\Phi_{ON}((1s^2, {}^1S, M_S = \ \ 0\ \{x_1x_2\})| \\ \langle\Phi_{ON}((1s^2, {}^3S, M_S = \ \ 0\ \{x_1x_2\})| \\ \langle\Phi_{ON}((1s^2, {}^3S, M_S = \ \ 1\ \{x_1x_2\})| \\ \langle\Phi_{ON}((1s^2, {}^3S, M_S = -1\ \{x_1x_2\})| \end{pmatrix}\\
&= \begin{pmatrix} 2^{-1/2} & -2^{-1/2} & 0 & 0 \\ 2^{-1/2} & 2^{-1/2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} \langle\Phi_{ON}((1s^2\ \{\ \ 1/2, -1/2\}\ \{x_1x_2\})| \\ \langle\Phi_{ON}((1s^2\ \{-1/2, \ \ 1/2\}\ \{x_1x_2\})| \\ \langle\Phi_{ON}((1s^2\ \{\ \ 1/2, \ \ 1/2\}\ \{x_1x_2\})| \\ \langle\Phi_{ON}((1s^2\ \{-1/2, -1/2\}\ \{x_1x_2\})| \end{pmatrix}
\end{aligned}$$

could be an illustration of (12) for bras.)

The columns of $(\mathbf{U})$ are labeled by $\{\Lambda_a\}\Lambda M$, where $\{\Lambda_a\}$ is an array of intermediate momenta, and the rows are labeled by the arrays $\{_N m\}$. Unitarity is expressed by the conditions [6]

$$\sum_{\{_N m\}} \left[\begin{array}{cccc} \lambda_1 & \ldots & \lambda_k & \Lambda \\ m_1 & \ldots & m_N & M \end{array} \right]^{\mathrm{A}}_{\{\Lambda_a\}} \left[\begin{array}{cccc} \lambda_1 & \ldots & \lambda_k & \Lambda' \\ m_1 & \ldots & m_N & M' \end{array} \right]^{\mathrm{A}}_{\{\Lambda'_a\}}$$
$$= \delta(\{\Lambda_a\}\Lambda M, \{\Lambda'_a\}\Lambda' M') \tag{13}$$

and

$$\sum_{\{\Lambda_a\}\Lambda M} \left[\begin{array}{cccc} \lambda_1 & \ldots & \lambda_k & \Lambda \\ m_1 & \ldots & m_N & M \end{array} \right]^{\mathrm{A}}_{\{\Lambda_a\}} \left[\begin{array}{cccc} \lambda_1 & \ldots & \lambda_k & \Lambda \\ m'_1 & \ldots & m'_N & M \end{array} \right]^{\mathrm{A}}_{\{\Lambda_a\}}$$
$$= \delta(\{_N m\}, \{_N m'\}) \ . \tag{14}$$

Another way of treating the equality (12) is that the basis (11) is used to form up a projection operator acting as identity operator in the space of functions (12), and the projection coefficients constitute a column of the matrix ($\mathbf{U}$):

$$\left|\Phi_{ON}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M\{_N x\})\right\rangle$$
$$= \left(\left|\Phi_{ON}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row} \times \left(\left\langle\Phi_{ON}(C^N\{_N m\}\{_N x\})\right|\right)_{column}$$
$$\times \left|\Phi_{ON}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M\{_N x\})\right\rangle \ . \tag{15}$$

But the basis (11) is non-physical one in the sense that the functions are nonantisymmetric. The direct antisymmetrization of it leads to a basis defined already by (8):

$$\widehat{\mathbf{A}}\left(\left|\Phi_{ON}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row}$$
$$= \left([N!]^{-1/2} \left\| \begin{array}{ccc} |\phi\,(n_1\lambda_1 m_1, x_1)\rangle & \ldots & |\phi\,(n_1\lambda_1 m_1, x_N)\rangle \\ \ldots & \ldots & \ldots \\ |\phi\,(n_i\lambda_k m_N, x_1)\rangle & \ldots & |\phi\,(n_i\lambda_k m_N, x_N)\rangle \end{array} \right\| \right\rangle \Bigg)_{row}$$
$$\left(\left|\Phi_{ON}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row} \ . \tag{16}$$

By applying this antisymmetrization to (12) and using the result in (9), we get

$$\left|\Phi_{ONA}(C^N \alpha\Lambda M\{_N x\})\right\rangle = \left(\prod_j N_j!\right)^{-1}$$
$$\times\left(\left|\Phi_{NA}(C^N\{_N m\}\{_N x\})\right\rangle\right)_{row}(\mathbf{U})(\mathbf{U}^T)\left(\left\langle\Phi_{NA}(C^N\{_N m\}\{_N x\})\right|\right)_{column}$$
$$\times\left|\Phi_{ONA}(C^N \alpha\Lambda M\{_N x\})\right\rangle$$
$$= \left(\prod_j N_j!\right)^{-1} \times \left(\left|\Phi_{NA}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M\{_N x\})\right\rangle\right)_{row}$$
$$\times\left(\left\langle\Phi_{NA}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M\{_N x\})\right|\right)_{column}$$
$$\times\left|\Phi_{ONA}(C^N \alpha\Lambda M\{_N x\})\right\rangle \ . \tag{17}$$

In SQR, the last formula is written as follows:

$$\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\left|0\right\rangle = \left(\prod_j N_j!\right)^{-1} \times \left(\widehat{\Phi}_{NA}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M)\left|0\right\rangle\right)_{row}$$
$$\times\left(\left\langle 0\right| \widehat{\Phi}^{\dagger}_{NA}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M)\right)_{column} \times \widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\left|0\right\rangle \ . \tag{18}$$

Formulas (17) or (18) are the expansions of the orthogonal, normalized to unity, and antisymmetric functions in terms of non-orthogonal, though also normalized to unity and antisymmetric functions. To make this expansion closer to a fractional parentage one, we need to relate somehow the basis (8) to the bases for configurations C^n and C^{N-n}. Let us do that.

First, we choose the coupling scheme A such that momenta Λ' and Λ'' corresponding to the configurations $C^n \equiv n_1\lambda_1^{n_1}\dots n_i\lambda_k^{n_k}$ and $C^{N-n} \equiv n_1\lambda_1^{N_1-n_1}\dots n_i\lambda_k^{N_k-n_k}$ are coupled in the last place:

$$\begin{bmatrix} \lambda_1 & \dots & \lambda_k & \Lambda \\ m_1 & \dots & m_N & M \end{bmatrix}^{\mathrm{A}}_{\{\Lambda_a\}} = \sum_{\{\Lambda'_a\}M'\{\Lambda''_a\}M''} \begin{bmatrix} \lambda_1 & \dots & \lambda_k & \Lambda' \\ m_1 & \dots & m_n & M' \end{bmatrix}^{\mathrm{A}'}_{\{\Lambda'_a\}}$$
$$\times \begin{bmatrix} \lambda_1 & \dots & \lambda_k & \Lambda'' \\ m_{n+1} & \dots & m_N & M'' \end{bmatrix}^{\mathrm{A}''}_{\{\Lambda''_a\}} \times \begin{bmatrix} \Lambda' & \Lambda'' & \Lambda \\ M' & M'' & M \end{bmatrix} , \tag{19}$$

with the coupling schemes A$'$ and A$''$ fixed. Then,

$$\begin{aligned}
&\left|\Phi_{NA}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M\{_N x\})\right\rangle \\
&\equiv \left|\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda', C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda'', \Lambda M\{_N x\})\right\rangle \\
&= \widehat{\mathbf{A}}\left|\left[\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda'\{_n x\}) \times \Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda''\{_{N-n} x\})\right]^{(\Lambda)}_{M}\right\rangle ,
\end{aligned} \tag{20}$$

where the antisymmetrizing operator $\widehat{\mathbf{A}}$ implies multiplication by an inverse square root of a binomial coefficient $[C_n^N]^{-1/2}$ and summation over all the possible (but arranged according to, say, ascending order of coordinate indexes each) nonoverlapping subarrays $\{_n x\}$ and $\{_{N-n} x\}$ constituting the array $\{_N x\} \equiv \{x_1 x_2 \dots x_N\}$ with proper phase factors.

Remembering that any odd permutation of coordinates $\{_N x\}$ changes the sign of antisymmetric function while even one does not, from (20) we infer that the overlap integrals on the rightmost of (17) obey the following:

$$\left\langle\Phi_{NA}(C^N, \mathrm{A}\{\Lambda_a\}, \Lambda M\{_N x\})\right| \Phi_{ONA}(C^N\alpha\Lambda M\{_N x\})\Big\rangle = [C_n^N]^{1/2}$$
$$\times\left\langle\left[\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda'\{_n x\}) \times \Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda''\{_{N-n} x\})\right]^{(\Lambda)}_{M}\right|$$
$$\times\left|\Phi_{ONA}(C^N\alpha\Lambda M\{_N x\})\right\rangle \ . \tag{21}$$

(Note that the order of coordinates in nonoverlapping subarrays $\{_n x\}$ and $\{_{N-n}x\}$ constituting $\{_N x\}$ may be arbitrary here.)

By putting (20) and (21) into (17) and applying the formula (17) itself for the wave functions of C^n and C^{N-n}, we get

$$\begin{aligned}
&\left|\Phi_{ONA}(C^N \alpha \Lambda_0 M_0 \{_N x\})\right\rangle \qquad (22)\\
&= \left(\prod_j C_{n_j}^{N_j}\right)^{-1} \sum_{\alpha'\Lambda'\alpha''\Lambda''\Lambda M} \left|\Phi_{NA}(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda'', \Lambda M\{_N x\})\right\rangle \\
&\times \left\langle \Phi_{NA}(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda'', \Lambda M\{_N x\})\right| \left.\Phi_{ONA}(C^N \alpha \Lambda_0 M_0 \{_N x\})\right\rangle \ .
\end{aligned}$$

(The derivation of formula (22) in detail is presented in the Appendix.) In SQR, expansion (22) is written down as

$$\begin{aligned}
&\widehat{\Phi}_{ONA}(C^N \alpha \Lambda_0 M_0) \left|0\right\rangle \qquad (23)\\
&= \left(\prod_j C_{n_j}^{N_j}\right)^{-1} \sum_{\alpha'\Lambda'\alpha''\Lambda''\Lambda M} \left[\widehat{\Phi}'_{ONA}(C^n\alpha'\Lambda') \times \widehat{\Phi}''_{ONA}(C^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_{M} \left|0\right\rangle \\
&\times \left\langle 0\right| \left\{\left[\widehat{\Phi}'_{ONA}(C^n\alpha'\Lambda') \times \widehat{\Phi}''_{ONA}(C^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_{M}\right\}^{\dagger} \widehat{\Phi}_{ONA}(C^N \alpha \Lambda_0 M_0) \left|0\right\rangle \ .
\end{aligned}$$

We note that the summation over ΛM in the expansions (22) and (23) is only formal since the integral (over $\{_N x\}$) at the rightmost of (22) or, correspondingly, the vacuum average on the right-hand side of (23) is just the matrix element of a C-number 1 independent of the z-projections of momenta due to Wigner-Eckart theorem and containing a $\delta(\Lambda_0 M_0, \Lambda M)$ [4]:

$$\begin{aligned}
&\left\langle \Phi_{NA}(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda'', \Lambda M\{_N x\})\right| \left.\Phi_{ONA}(C^N \alpha \Lambda_0 M_0 \{_N x\})\right\rangle \\
&= \left\langle 0\right| \left\{\left[\widehat{\Phi}'_{ONA}(C^n\alpha'\Lambda') \times \widehat{\Phi}''_{ONA}(C^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_{M}\right\}^{\dagger} \widehat{\Phi}_{ONA}(C^N \alpha \Lambda M) \left|0\right\rangle \\
&= [2\Lambda+1]^{-1/2} \begin{bmatrix} \Lambda_0 & 0 & \Lambda \\ M_0 & 0 & M \end{bmatrix} \left\langle C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda'', \Lambda M \right\| \left. C^N \alpha \Lambda_0 M_0 \right\rangle \\
&= [2\Lambda+1]^{-1/2}\, \delta(\Lambda_0 M_0, \Lambda M) \qquad (24)\\
&\times \left\langle C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda'', \Lambda M \right\| \left. C^N \alpha \Lambda_0 M_0 \right\rangle \ .
\end{aligned}$$

Thus, we have obtained an expansion that in a single-shell case is similar to the conventional CFPs expansion for a single-shell case:

$$\begin{aligned}
&\left|\Phi_{ONA}(\lambda^N \alpha \Lambda M \{_N x\})\right\rangle \\
&= \sum_{\alpha'\Lambda'\alpha''\Lambda''} \left|\left[\Phi'_{ONA}(\lambda^n\alpha'\Lambda'\{_n x\}) \times \Phi''_{ONA}(\lambda^{N-n}\alpha''\Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_{M}\right\rangle \qquad (25)\\
&\times \left\langle \left[\Phi'_{ONA}(\lambda^n\alpha'\Lambda'\{_n x\}) \times \Phi''_{ONA}(\lambda^{N-n}\alpha''\Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_{M} \right| \left.\Phi_{ONA}(\lambda^N \alpha \Lambda M \{_N x\})\right\rangle
\end{aligned}$$

(only simple antisymmetrization in (25) compared to (22) is missing). However, the expansion (22) in many-shell case is simpler than the (antisymmetrized) standard CFPs expansion for inequivalent electrons case [7], expressed as

$$\begin{aligned}
&\left|\Phi_{ONA}(C^N\alpha\Lambda M\{_Nx\})\right\rangle \\
&= \sum_{n_1\ldots n_k}\sum_{\alpha'\Lambda'\alpha''\Lambda''}\left|\left[\Phi'_{ONA}(C^n\alpha'\Lambda'\{_nx\})\times\Phi''_{ONA}(C^{N-n}\alpha''\Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_M\right\rangle \qquad (26)\\
&\times\left\langle\left[\Phi'_{ONA}(C^n\alpha'\Lambda'\{_nx\})\times\Phi''_{ONA}(C^{N-n}\alpha''\Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_M \mid \Phi_{ONA}(C^N\alpha\Lambda M\{_Nx\})\right\rangle ,
\end{aligned}$$

because the former does not contain the sum $\sum_{n_1\ldots n_k}$ (with $n_1+\ldots+n_k=n$) over all the possible distributions of N electrons in k shells of two mutually nonantisymmetrized functions Φ' and Φ'' for n and $(N-n)$ electrons (i.e., over all the configurations for parent terms). Note that the last integral in (26) (the brackets "$\langle\ \rangle$" imply integration over spatial coordinates $\{_Nx\}$, of course; the spin variables belong to the array $\{_Nm\}$) is the conventional many-shell CFP.

So, the consequent usage of antisymmetrized functions' bases (which is equivalent to SQR) led us to formula (23). Though the latter differs from the "real" fractional parentage expansion (26), still, the words "fractional parentage" are applicable. One may notice that the "parents" are still well defined and, moreover, that there remain **only two** configurations for parent terms.

3. Properties of the New Expansion Coefficients

The relationship between the new expansion coefficients (see (22) and (23)) and the conventional many-shell CFPs (see (26)) may be easily established by antisymmetrizing the wave functions on the left part of the former ones. They turn out to be just simply proportional. As in (21), we have

$$\begin{aligned}
&\langle 0|\left\{\left[\widehat{\Phi}'_{ONA}(C^n\alpha'\Lambda')\times\widehat{\Phi}''_{ONA}(C^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_M\right\}^{\dagger}\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\,|0\rangle \qquad (27)\\
&= \left\langle\Phi_{NA}(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda'', \Lambda M\{_Nx\})\right|\left.\Phi_{ONA}(C^N\alpha\Lambda M\{_Nx\})\right\rangle = [C^N_n]^{1/2}\\
&\times\left\langle\left[\Phi'_{ONA}(C^n\alpha'\Lambda'\{_nx\})\times\Phi''_{ONA}(C^{N-n}\alpha''\Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_M \mid \Phi_{ONA}(C^N\alpha\Lambda M\{_Nx\})\right\rangle .
\end{aligned}$$

Now, let us introduce the quantities defined as follows:

$$\begin{aligned}
&\left(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda''\right\|\left. C^N\alpha\Lambda\right) \equiv \left(\prod_j C^{N_j}_{n_j}\right)^{-1/2}\\
&\times\langle 0|\left\{\left[\widehat{\Phi}'_{ONA}(C^n\alpha'\Lambda')\times\widehat{\Phi}''_{ONA}(C^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_M\right\}^{\dagger}\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\,|0\rangle\\
&= \langle 0|\left\{\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\right\}^{\dagger}\left[\widehat{\Phi}'_{ONA}(C^n\alpha'\Lambda')\times\widehat{\Phi}''_{ONA}(C^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_M|0\rangle
\end{aligned}$$

$$\times\left(\prod_j C_{n_j}^{N_j}\right)^{-1/2} . \tag{28}$$

They are independent of M and orthonormal, as is implied by (22) and (23):

$$\begin{aligned}&\sum_{\alpha'\Lambda'\alpha''\Lambda''}\left(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda''\right\| C^N\alpha\Lambda\Big)\left(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda''\right\| C^N\alpha_0\Lambda_0\Big)\\&\times\delta(\Lambda,\Lambda_0)\\&=\langle 0|\left\{\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\right\}^\dagger\widehat{\Phi}_{ONA}(C^N\alpha_0\Lambda_0 M)\,|0\rangle\\&=\delta(\alpha\Lambda,\alpha_0\Lambda_0)\ ,\end{aligned}\tag{29}$$

just like the ordinary single-shell CFPs from (25) are. Moreover, they are equal to CFPs in a single-shell case:

$$\begin{aligned}&\left(\lambda^n\alpha'\Lambda',\lambda^{N-n}\alpha''\Lambda''\right\|\lambda^N\alpha\Lambda\Big)\equiv\left(C_n^N\right)^{-1/2}\\&\times\langle 0|\left\{\left[\widehat{\Phi}'_{ONA}(\lambda^n\alpha'\Lambda')\times\widehat{\Phi}''_{ONA}(\lambda^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_M\right\}^\dagger\widehat{\Phi}_{ONA}(\lambda^N\alpha\Lambda M)\,|0\rangle\\&=\left(C_n^N\right)^{-1/2}\left\langle\Phi_{NA}(\lambda^n\alpha'\Lambda',\lambda^{N-n}\alpha''\Lambda'',\Lambda M\{_N x\})\right|\Phi_{ONA}(\lambda^N\alpha\Lambda_0 M_0\{_N x\})\Big\rangle\\&=\Big\langle\left[\Phi'_{ONA}(\lambda^n\alpha'\Lambda'\{_n x\})\times\Phi''_{ONA}(\lambda^{N-n}\alpha''\Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_M|\ \Phi_{ONA}(\lambda^N\alpha\Lambda M\{_N x\})\Big\rangle\ ,\end{aligned}\tag{30}$$

as follows from (27). Thus, one has good reasons to give the quantities (28) a name "CFPs". Hereafter, we will call them "new CFPs", referring to the CFPs from (26) as "conventional CFPs".

Now we see from (23) or, alternatively, from

$$\begin{aligned}&\widehat{\Phi}_{ONA}(C^N\alpha\Lambda M)\,|0\rangle\\&=\sum_{\alpha'\Lambda'\alpha''\Lambda''}\left(\prod_j C_{n_j}^{N_j}\right)^{-1/2}\left[\widehat{\Phi}'_{ONA}(C^n\alpha'\Lambda')\times\widehat{\Phi}''_{ONA}(C^{N-n}\alpha''\Lambda'')\right]^{(\Lambda)}_M|0\rangle\\&\times\left(C^n\alpha'\Lambda',C^{N-n}\alpha''\Lambda''\right\|C^N\alpha\Lambda\Big)\end{aligned}\tag{31}$$

that Fano [8] has not been absolutely right in stating that the use of coefficients of fractional parentage for mixed configurations provides few simplifications to the usual techniques. The simplification achieved is the consequence of automatical antisymmetry of the wave functions in the SQR . In the new approach, one needs a considerably smaller quantity of standard parameters (i.e., new CFPs) to construct a basis. For example, single-electron CFPs $(p,p^4d^2||p^5d^2)$ **and** $(d,p^5d||p^5d^2)$ or two-electron CFPs $(p^2,p^3d^2||p^5d^2)$ **and** $(pd,p^4d||p^5d^2)$ **and** $(d^2,p^5||p^5d^2)$ are needed to build up a basis for p^5d^2 in the conventional CFPs approach. In a sense, the parameters mentioned are no longer the coefficients of fractional parentage, because no antisymmetrization is performed that is essential in the definition of the conventional CFPs. The new expansion coefficients only orthonormalize an overdetermined basis. Nevertheless, we stress once more that we prefer the name "coefficients of fractional parentage", due to the fact that the "parents" are still well defined.

With CFPs being defined in SQR, quasispin and isospin methods [4] can be easily and transparently applied to investigate their properties. The usage of quasispin and its z-projection operators' eigenfunctions allows one to factorize a CFP and express it as the product of the Clebsch-Gordan coefficient of the quasispin group $\mathrm{SU}(2)^Q$ and a reduced CFP independent of the quasispin z-projections' quantum numbers. The factorization of the matrix elements of the sums of Racah's unitary tensor operators [9] $\sum u_i^k \equiv U^k$ and $\sum v_i^{k1} \equiv V^{k1}$ can also be performed. Thus, the reduced CFPs in such an approach are the main standard quantities to be tabulated for further use in analysis of the matrix elements of operators under investigation. Also, the extension of tables of reduced CFPs is considerably smaller than that of CFPs. The similar factorization is applicable when isospin formalism for the electronic configurations $n_1\lambda^{N_1}n_2\lambda^{N_2}$ is used. Then, the two electronic shells are treated as one shell $\lambda^{N_1+N_2}$; isospin and its z-projection operators' eigenfunctions with different isospin z-projection eigenvalues $M_T = (N_2 - N_1)/2$ correspond to different distributions of electrons between the shells. For the configurations mentioned, the isospin formalism can be combined with quasispin formalism, together forming up the five-dimensional quasispin formalism [10]. The formulas and examples illustrating these formalisms and properties of CFPs can be found in [4, 11, 12].

Still, one more useful property of the CFPs is to be pointed out. In SQR, the hole representation is easy to introduce. For the CFPs defined by (28), a hole representation of any shell is equivalent to Hermitian conjugation of that part of operator between bra and ket vacuum states which corresponds to that particular shell. The vacuum state of that shell is filled up with particles then, but its tensorial properties in Λ space remain invariant. Therefore, the numerical value of a CFP is not affected by such a change of representation. For example,

$$(pd\Lambda', p||p^2d\alpha\Lambda) = (\bar{p}d\Lambda', \bar{p}||\bar{p}^2d\alpha\Lambda) \ , \tag{32}$$

which is not obvious from the point of view of CR, where configurations for parent terms with number of particles $N \leq 0$ are not easy to imagine.

In the next section, we derive some properties of CFPs by considering the overlap integrals of wave functions.

4. Bilinear Combinations of CFPs

The numerical values of the new CFPs could be obtained recurrently according to the formulas that are analogous to the known Redmond's formula [13] for the single-shell case. In the many-shell case, the necessary formulas in SQR are obtained applying the method proposed for single-shell case by Judd [14], namely, the matrix elements of the operators present in the explicit form of the commutator

$$\left[\left\{\widehat{\Psi}_1'(C^n\alpha_1'\Lambda_1')\right\}^\dagger, \widehat{\Psi}_2'(C^n\alpha_2'\Lambda_2')\right] \ , \tag{33}$$

determined in the basis of functions $\widehat{\Psi}(C^N\alpha\Lambda)\,|0\rangle$, are expressed via bilinear combinations of CFPs of the types $\left(C^n, C^N \middle\| C^{N+n}\right)$ and $\left(C^n, C^{N-n} \middle\| C^N\right)$. In there, the numerical values of CFPs with $\sum(N_i + n_i) = N + n$ electrons in the final state are determined by those of CFPs with $\sum N_i = N$ electrons in the final state. The application of such a recurrent relationship requires one to define the initial values of CFPs. These are determined from the same recurrent relationship remembering that for $N_i - n_i < 0$ a CFP $\left(C^n C^{N-n} \middle\| C^N\right)$ does not make sense and has to be equal to zero.

Let us consider, e.g., a two-shell two-electron CFP [15]. We introduce the operator of creation of a normalized two-shell two-electron function of coupled momenta:

$$A^{(k)}_q\,|0\rangle \equiv \left[b^{(\lambda_2)} \times a^{(\lambda_1)}\right]^{(k)}_q |0\rangle \equiv |n_1\lambda_1 n_2\lambda_2, kq\rangle \equiv \left|C^2 kq\right\rangle \ . \tag{34}$$

From standard anticommutation of $b^{(\lambda_2)}$ and $a^{(\lambda_1)}$ and properties of irreducible tensors (see [4])

$$\tilde{a}^{(\lambda_1)}_m = (-1)^{\lambda_1 - m} a^{(\lambda_1)\dagger}_{-m} \ , \tilde{b}^{(\lambda_2)}_m = (-1)^{\lambda_2 - m} b^{(\lambda_2)\dagger}_{-m} \ , \tag{35}$$

we get (where $[\lambda_i, \lambda_j, \ldots] \equiv \dim(\lambda_i) \times \dim(\lambda_j)\ldots$)

$$\begin{aligned}
&\left[A^{(k')\dagger}_{q'}, A^{(k)}_q\right] = \delta(kq, k'q') - \sum_{\mathcal{K}} (-1)^{\lambda_2 - \lambda_1 + q'} \sqrt{[k, k']} \\
&\times \begin{bmatrix} k' & k & \mathcal{K} \\ -q' & q & q - q' \end{bmatrix} \left[\begin{Bmatrix} \lambda_1 & \lambda_1 & \mathcal{K} \\ k' & k & \lambda_2 \end{Bmatrix} \left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})}_{q-q'} \right. \\
&\left. + (-1)^{k+k'} \begin{Bmatrix} \lambda_2 & \lambda_2 & \mathcal{K} \\ k' & k & \lambda_1 \end{Bmatrix} \left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\mathcal{K})}_{q-q'} \right] \ .
\end{aligned} \tag{36}$$

Let three complete sets of orthonormal two-shell wave functions in SQR be defined:

$$\widehat{\varphi}_{-1}(n_1\lambda_1^{N_1-1} n_2\lambda_2^{N_2-1}\alpha_{-1}\Lambda_{-1}M_{-1})\,|0\rangle \equiv \left|C^{N-2}\alpha_{-1}\Lambda_{-1}M_{-1}\right\rangle \ , \tag{37}$$

$$\widehat{\varphi}_0(n_1\lambda_1^{N_1} n_2\lambda_2^{N_2}\alpha_0\Lambda_0M_0)\,|0\rangle \equiv \left|C^N\alpha_0\Lambda_0M_0\right\rangle \ , \tag{38}$$

$$\widehat{\varphi}_1(n_1\lambda_1^{N_1+1} n_2\lambda_2^{N_2+1}\alpha_1\Lambda_1M_1)\,|0\rangle \equiv \left|C^{N+2}\alpha_1\Lambda_1M_1\right\rangle \ . \tag{39}$$

According to (23) the wave functions from an overdetermined basis,

$$\left|C^{N+2}, k, \alpha_0\Lambda_0, \Lambda_1M_1\right\rangle \equiv \left[A^{(k)} \times \left|C^N\alpha_0\Lambda_0\right\rangle\right]^{(\Lambda_1)}_{M_1} \tag{40}$$

can be transformed to make a basis (39):

$$\begin{aligned}
\left|C^{N+2}\alpha_1\Lambda_1M_1\right\rangle &= \frac{1}{(N_1+1)(N_2+1)} \sum_{k\alpha_0\Lambda_0} \left[A^{(k)} \times \left|C^N\alpha_0\Lambda_0\right\rangle\right]^{(\Lambda_1)}_{M_1} \\
&\times \left(\left[A^{(k)} \times \left|C^N\alpha_0\Lambda_0\right\rangle\right]^{(\Lambda_1)}_{M_1}\right)^\dagger \left|C^{N+2}\alpha_1\Lambda_1M_1\right\rangle \ .
\end{aligned} \tag{41}$$

Let us investigate the overlap matrix defined in the basis (40):

$$
\begin{aligned}
S_1 &= \left\langle C^{N+2}, k', \alpha_0'\Lambda_0', \Lambda_1 M_1 \mid C^{N+2}, k, \alpha_0\Lambda_0, \Lambda_1 M_1 \right\rangle \\
&= \left(\left[A^{(k')} \times \left| C^N \alpha_0'\Lambda_0' \right\rangle \right]^{(\Lambda_1)}_{M_1} \right)^{\dagger} \left[A^{(k)} \times \left| C^N \alpha_0\Lambda_0 \right\rangle \right]^{(\Lambda_1)}_{M_1} .
\end{aligned} \tag{42}
$$

The rows and columns of this matrix are labeled by different arrays of $k, \alpha_0\Lambda_0$, and Λ_1. It is diagonal with respect to Λ_1 and does not depend upon M_1.

By applying projector onto the complete orthonormal basis (39), from (42) we get

$$
\begin{aligned}
S_1 &= \sum_{\alpha''} \left(\left[A^{(k')} \times \left| C^N \alpha_0'\Lambda_0' \right\rangle \right]^{(\Lambda_1)}_{M_1} \right)^{\dagger} \left| C^{N+2} \alpha'' \Lambda_1 M_1 \right\rangle \\
&\times \left\langle C^{N+2} \alpha'' \Lambda_1 M_1 \right| \left[A^{(k)} \times \left| C^N \alpha_0\Lambda_0 \right\rangle \right]^{(\Lambda_1)}_{M_1} .
\end{aligned} \tag{43}
$$

Then, we commute $A^{(k')\dagger}_{q'}$ and $A^{(k)}_{q}$ in (42) according to (36) and apply the projector onto the basis (37). After those transformations, we get

$$
\begin{aligned}
S_1 &= \delta(k\alpha_0\Lambda_0, k\alpha_0'\Lambda_0') + \sum_{\alpha\Lambda} (-1)^{k+k'+\Lambda_0+\Lambda_0'} \sqrt{[\Lambda_0, \Lambda_0']} \\
&\times \left\{ \begin{array}{ccc} k' & \Lambda_0' & \Lambda_1 \\ k & \Lambda_0 & \Lambda \end{array} \right\} \left\langle C^N \alpha_0'\Lambda_0' M_0' \right| \left[A^{(k)} \times \left| C^{N-2} \alpha\Lambda \right\rangle \right]^{(\Lambda_0')}_{M_0'} \\
&\times \left(\left\langle C^N \alpha_0\Lambda_0 M_0 \right| \left[A^{(k')} \times \left| C^{N-2} \alpha\Lambda \right\rangle \right]^{(\Lambda_0)}_{M_0} \right)^{\dagger} \\
&- \sum_{\mathcal{K}} (-1)^{\lambda_2-\lambda_1+k+k'+\mathcal{K}-\Lambda_0'-\Lambda_1} \sqrt{[k, k', \mathcal{K}]} \left\{ \begin{array}{ccc} k & k' & \mathcal{K} \\ \Lambda_0' & \Lambda_0 & \Lambda_1 \end{array} \right\} \\
&\times \left[\left\{ \begin{array}{ccc} \lambda_1 & \lambda_1 & \mathcal{K} \\ k' & k & \lambda_2 \end{array} \right\} \left(C^N \alpha_0'\Lambda_0' \middle\| \left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)} \right]^{(\mathcal{K})} \middle\| C^N \alpha_0\Lambda_0 \right) \right. \\
&\left. + (-1)^{k+k'} \left\{ \begin{array}{ccc} \lambda_2 & \lambda_2 & \mathcal{K} \\ k' & k & \lambda_1 \end{array} \right\} \left(C^N \alpha_0'\Lambda_0' \middle\| \left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)} \right]^{(\mathcal{K})} \middle\| C^N \alpha_0\Lambda_0 \right) \right] .
\end{aligned} \tag{44}
$$

From (43), (44), and remembering (28), finally we get the recurrent relationship for the two-shell two-particle CFPs:

$$
\begin{aligned}
&\sum_{\alpha''} (N_2+1)(N_1+1) \left(C^2 k', C^N \alpha_0'\Lambda_0' \middle\| C^{N+2} \alpha'' \Lambda_1 \right) \left(C^2 k, C^N \alpha_0\Lambda_0 \middle\| C^{N+2} \alpha'' \Lambda_1 \right) \\
&= \delta(k\alpha_0\Lambda_0, k'\alpha_0'\Lambda_0') + \sum_{\alpha\Lambda} (-1)^{k+k'+\Lambda_0+\Lambda_0'} \, N_2 \, N_1 \, \sqrt{[\Lambda_0, \Lambda_0']} \left\{ \begin{array}{ccc} k' & \Lambda_0' & \Lambda_1 \\ k & \Lambda_0 & \Lambda \end{array} \right\} \\
&\times \left(C^2 k, C^{N-2} \alpha\Lambda \middle\| C^N \alpha_0'\Lambda_0' \right) \left(C^2 k', C^{N-2} \alpha\Lambda \middle\| C^N \alpha_0\Lambda_0 \right) \\
&- \sum_{\mathcal{K}} (-1)^{\lambda_2-\lambda_1+k+k'+\mathcal{K}-\Lambda_0'-\Lambda_1} \sqrt{[k, k', \mathcal{K}]} \left\{ \begin{array}{ccc} k & k' & \mathcal{K} \\ \Lambda_0' & \Lambda_0 & \Lambda_1 \end{array} \right\}
\end{aligned}
$$

$$\times \left[\left\{ \begin{array}{ccc} \lambda_1 & \lambda_1 & \mathcal{K} \\ k' & k & \lambda_2 \end{array} \right\} \left(C^N \alpha_0' \Lambda_0' \left\| \left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)} \right]^{(\mathcal{K})} \right\| C^N \alpha_0 \Lambda_0 \right) \right. \tag{45}$$
$$\left. + (-1)^{k+k'} \left\{ \begin{array}{ccc} \lambda_2 & \lambda_2 & \mathcal{K} \\ k' & k & \lambda_1 \end{array} \right\} \left(C^N \alpha_0' \Lambda_0' \left\| \left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)} \right]^{(\mathcal{K})} \right\| C^N \alpha_0 \Lambda_0 \right) \right] .$$

In this relationship, the submatrix elements of irreducible tensor operators $\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})}_Q$ and $\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\mathcal{K})}_Q$ in the basis of two-shell wave functions appear. Let us suppose that for one shell empty ($N_i = 0$ for any i) the functions $\left|C^N \alpha_0 \Lambda_0 M_0\right\rangle$ of the basis (38) coincide with the functions of the conventional single-shell basis. Then, those submatrix elements are proportional to the tabulated quantities $\left(l^N, \alpha'\Lambda' \right\| U^\kappa \left\| l^N, \alpha\Lambda\right)$ and $\left(l^N, \alpha'\Lambda' \right\| V^{\kappa 1} \left\| l^N, \alpha\Lambda\right)$ (we reproduce here the ones presented in LS coupling in [16]) :

$$\left(l^N, \alpha' L' S' \left\| \left[c^{(ls)} \times \tilde{c}^{(ls)} \right]^{(00)} \right\| l^N, \alpha L S \right)$$
$$= -\delta(\alpha L S, \alpha' L' S') \sqrt{\frac{[L,S]}{[l,s]}} ,$$

$$\left(l^N, \alpha' L' S' \left\| \left[c^{(ls)} \times \tilde{c}^{(ls)} \right]^{(10)} \right\| l^N, \alpha L S \right)$$
$$= -\delta(\alpha L S, \alpha' L' S') \sqrt{\frac{3[L,S]L(L+1)}{[l,s]l(l+1)}} ,$$

$$\left(l^N, \alpha' L' S' \left\| \left[c^{(ls)} \times \tilde{c}^{(ls)} \right]^{(\kappa 0)} \right\| l^N, \alpha L S \right)$$
$$= -\sqrt{\frac{[\kappa]}{2}} \left(l^N, \alpha' L' S' \right\| U^\kappa \left\| l^N, \alpha L S \right) ,$$

$$\left(l^N, \alpha' L' S' \left\| \left[c^{(ls)} \times \tilde{c}^{(ls)} \right]^{(01)} \right\| l^N, \alpha L S \right)$$
$$= -\delta(\alpha L S, \alpha' L' S') \sqrt{\frac{2[L,S]S(S+1)}{[l]}} ,$$

$$\left(l^N, \alpha' L' S' \left\| \left[c^{(ls)} \times \tilde{c}^{(ls)} \right]^{(\kappa 1)} \right\| l^N, \alpha L S \right)$$
$$= -\sqrt{2[\kappa]} \left(l^N, \alpha' L' S' \right\| V^{\kappa 1} \left\| l^N, \alpha L S \right) ; \tag{46}$$

here l denotes l_1 or l_2, and $c^{(ls)}$ denotes $a^{(l_1 s)}$or $b^{(l_2 s)}$.

One can obtain recurrent relationships for the submatrix elements of $\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})}$ and $\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\mathcal{K})}$ in the basis of two-shell wave functions. By using the fact that the functions of basis considered are the eigenfunctions of occupation number operators $\widehat{N}_1$ and $\widehat{N}_2$ [4],

$$\widehat{N}_1 = -\sqrt{[\lambda_1]}\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(0)} \quad , \quad \widehat{N}_2 = -\sqrt{[\lambda_2]}\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(0)} \quad , \tag{47}$$

and by applying Wigner-Eckart theorem in the form of (3.41) of [4] for submatrix elements of $\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})}_Q$ and $\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\mathcal{K})}_Q$, we get that, e.g.,

$$\begin{aligned}
&\left(C^{N+2}\alpha_1'\Lambda_1' \left\| \left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})} \right\| C^{N+2}\alpha_1\Lambda_1\right) = \frac{(-1)^{2\mathcal{K}+1}}{N_2+1}\sqrt{\frac{[\lambda_2]}{[\Lambda_1']}} \\
&\times \sum_{M_1 Q M_1'} \left\langle C^{N+2}\alpha_1'\Lambda_1' M_1' \left| \left[\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})} \right.\right.\right. \\
&\times \left.\left.\left. \left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(0)}\right]^{(\mathcal{K})}_Q \right| C^{N+2}\alpha_1\Lambda_1 M_1 \right\rangle \left[\begin{array}{ccc} \Lambda_1 & \mathcal{K} & \Lambda_1' \\ M_1 & Q & M_1' \end{array}\right] .
\end{aligned} \tag{48}$$

The standard methods of angular momentum theory [6] allow one to obtain

$$\begin{aligned}
&\left[\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})} \times \left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(0)}\right]^{(\mathcal{K})}_Q \\
&= \sum_{kq\mathcal{K}_1 Q_1} (-1)^{\lambda_1+\lambda_2+k+\mathcal{K}+1} \sqrt{\frac{[k,\mathcal{K}_1]}{[\lambda_2]}} \left\{\begin{array}{ccc} \lambda_1 & \lambda_1 & \mathcal{K} \\ \mathcal{K}_1 & k & \lambda_2 \end{array}\right\} \left[\begin{array}{ccc} k & \mathcal{K}_1 & \mathcal{K} \\ q & Q_1 & Q \end{array}\right] \\
&\times \left[b^{(\lambda_2)} \times a^{(\lambda_1)}\right]^{(k)}_q \cdot \left[\tilde{b}^{(\lambda_2)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K}_1)}_{Q_1} .
\end{aligned} \tag{49}$$

By putting (49) into (48), using the projector onto basis (39) and remembering (28), we express the right side of (48) as the bilinear combination of CFPs. Then, we have

$$\begin{aligned}
&\left(C^{N+2}\alpha_1'\Lambda_1' \left\| \left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})} \right\| C^{N+2}\alpha_1\Lambda_1\right) \\
&= (N_1+1) \sum_{k\mathcal{K}_1\alpha_0'\Lambda_0'} (-1)^{\lambda_2-\lambda_1-\Lambda_1-\Lambda_0'} \sqrt{[k,\mathcal{K},\mathcal{K}_1,\Lambda_1,\Lambda_1']} \left\{\begin{array}{ccc} \Lambda_1 & \Lambda_0' & \mathcal{K}_1 \\ k & \mathcal{K} & \Lambda_1' \end{array}\right\} \\
&\times \left\{\begin{array}{ccc} \lambda_2 & \lambda_1 & \mathcal{K}_1 \\ \mathcal{K} & k & \lambda_1 \end{array}\right\} \left(C^2 k, C^N\alpha_0'\Lambda_0' \,\|\, C^{N+2}\alpha_1'\Lambda_1'\right) \left(C^2\mathcal{K}_1, C^N\alpha_0'\Lambda_0' \,\|\, C^{N+2}\alpha_1\Lambda_1\right) .
\end{aligned} \tag{50}$$

An analogous expression is valid for the submatrix elements of $\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\mathcal{K})}_Q$:

$$\begin{aligned}
&\left(C^{N+2}\alpha_1'\Lambda_1' \left\| \left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\mathcal{K})} \right\| C^{N+2}\alpha_1\Lambda_1\right) = (N_2+1) \\
&\times \sum_{k\mathcal{K}_1\alpha_0'\Lambda_0'} (-1)^{\lambda_2-\lambda_1-k+\mathcal{K}_1+\Lambda_1+\Lambda_0'} \sqrt{[k,\mathcal{K},\mathcal{K}_1,\Lambda_1,\Lambda_1']} \left\{\begin{array}{ccc} \Lambda_1 & \Lambda_0' & \mathcal{K}_1 \\ k & \mathcal{K} & \Lambda_1' \end{array}\right\} \\
&\times \left\{\begin{array}{ccc} \lambda_1 & \lambda_2 & \mathcal{K}_1 \\ \mathcal{K} & k & \lambda_2 \end{array}\right\} \left(C^2 k, C^N\alpha_0'\Lambda_0' \,\|\, C^{N+2}\alpha_1'\Lambda_1'\right) \left(C^2\mathcal{K}_1, C^N\alpha_0'\Lambda_0' \,\|\, C^{N+2}\alpha_1\Lambda_1\right) .
\end{aligned} \tag{51}$$

The system of relationships (45), (50), and (51) obtained allows one to determine the numerical values of two-shell two-particle CFPs in a recurrent way. However, the unambiguous values of two-shell two-particle CFPs and submatrix elements of tensor operators $\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\mathcal{K})}_Q$ and $\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\mathcal{K})}_Q$ are possible to determine only when repeating terms Λ for configuration C^{N+2} do not occur. It is clear that with the occurrence of $K > 1$ times repeating terms Λ_1 the numerical value of the right-hand side of (45) is well defined, but the summation over α'' on the left-hand side,

$$\sum_{\alpha''} \left(C^2 k', C^N \alpha_0' \Lambda_0' \parallel C^{N+2} \alpha'' \Lambda_1\right) \left(C^2, C^N \alpha_0 \Lambda_0 \parallel C^{N+2} \alpha'' \Lambda_1\right) \ , \tag{52}$$

does not disappear. If one treats a system of CFPs for a repeating Λ_1 as an array of $r = \dim(k) \cdot \dim(\alpha_0 \Lambda_0)$ vectors having the same origin in the K-dimensional space, then (45) defines only the length of those vectors and angles between them but never the lengths of their projections onto K mutually orthogonal coordinate axes (with their orientation in that space being undefined). The numerical values of two-shell two-electron CFPs should be treated then as the above-mentioned lengths of projections; therefore, they are determined by (45) only to the exactness of an orthogonal transformation characterized by $K(K-1)/2$ free parameters.

Among others, the easiest (and the most general) way to eliminate the ambiguities is to ascribe numerical value zero to certain $K(K-1)/2$ CFPs. The numerical values of CFPs $(pd\ L_1 S_1,\ d\ L_2 S_2 \|\ pd^2\ \alpha LS)$ obtained from recurrent relationship (45) were fixed in such a way (see Table 1).

Alongside relations of the type of (45), (50), and (51), still more relations for the bilinear combinations of CFPs can be obtained in an easy way. One just needs to exploit the fact that the wave functions of the bases where CFPs are defined are just the eigenfunctions of certain operators by their definition. For example, the wave functions $\widehat{\Psi}\left(\lambda^{N_1} \ldots \lambda^{N_k} \alpha L S M_L M_S\right) |0\rangle$ are the eigenfunctions of $\widehat{N}_1 \ldots \widehat{N}_k, S^{(1)}_q, L^{(1)}_q$ and of their sums and products. By expressing the matrix elements of such tensor operators in SQR via bilinear combinations of CFPs, on the one hand, and via their eigenvalues, on the other, we get a system of linear algebraic equations for the bilinear combinations of CFPs. In some cases, it is easy to solve these systems and to obtain explicit expressions for simpler bilinear combinations of CFPs (say, for those not containing summation over the spin-type quantum numbers, as in [17]).

Let us obtain a series of such relationships for two-shell two-particle CFPs in LS-coupling scheme. We limit ourselves to the operators $\widehat{N} \cdot \widehat{N}$, $(S^{(1)} \cdot S^{(1)})$, $\widehat{S}^2$ and $\widehat{N} \cdot S^{(1)}$. By considering the eigenvalues of these operators [4], writing down in irreducible tensor form

$$\widehat{N} = \widehat{N}_1 + \widehat{N}_2 = -\sqrt{[\lambda_1]} \left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(0)}_0 - \sqrt{[\lambda_2]} \left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(0)}_0 \ , \tag{53}$$

Table 1. CFPs $(pd\ L_1S_1,\ d\ L_2S_2 \parallel pd^2\ \alpha LS)$.

${}^{2S+1}L^{\alpha}$		^{2}S	^{2}P^0	^{2}P^1	^{2}P^2	^{2}D^0	^{2}D^1	^{2}D^2
${}^{2S+1}L_1$	${}^{2S+1}L_2$							
${}^1P$	${}^2D$		$\frac{-\sqrt{19}}{2\sqrt{10}}$	0	0	$\frac{-\sqrt{23}}{2\sqrt{10}}$	0	0
${}^3P$			$\frac{\sqrt{3}}{2\sqrt{10\cdot19}}$	$\frac{3\sqrt{11}}{\sqrt{10\cdot19}}$	0	$\frac{-3\sqrt{3}}{2\sqrt{10\cdot23}}$	$\frac{\sqrt{7\cdot13}}{\sqrt{10\cdot23}}$	0
${}^1D$		$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}}{2\sqrt{2\cdot19}}$	$\frac{-5}{\sqrt{22\cdot19}}$	$\frac{\sqrt{7}}{\sqrt{33}}$	$\frac{-\sqrt{7}}{2\sqrt{2\cdot23}}$	$\frac{5\sqrt{3}}{\sqrt{26\cdot23}}$	$\frac{\sqrt{6}}{\sqrt{13}}$
${}^3D$		$\frac{1}{2}$	$\frac{3}{2\sqrt{2\cdot19}}$	$\frac{2\sqrt{2}}{\sqrt{33\cdot19}}$	$\frac{-\sqrt{7}}{\sqrt{11}}$	$\frac{-\sqrt{21}}{2\sqrt{2\cdot23}}$	$\frac{-4\sqrt{2}}{\sqrt{13\cdot23}}$	$\frac{\sqrt{2}}{\sqrt{13}}$
${}^1F$			$\frac{\sqrt{21}}{\sqrt{10\cdot19}}$	$\frac{-\sqrt{70}}{\sqrt{11\cdot19}}$	$\frac{-\sqrt{5}}{2\sqrt{33}}$	$\frac{-\sqrt{7}}{\sqrt{5\cdot23}}$	$\frac{2\sqrt{15}}{\sqrt{13\cdot23}}$	$\frac{-\sqrt{15}}{2\sqrt{13}}$
${}^3F$			$\frac{3\sqrt{7}}{\sqrt{10\cdot19}}$	$\frac{4\sqrt{14}}{\sqrt{15\cdot11\cdot19}}$	$\frac{\sqrt{5}}{2\sqrt{11}}$	$\frac{-\sqrt{21}}{\sqrt{5\cdot23}}$	$\frac{-16}{\sqrt{65\cdot23}}$	$\frac{-\sqrt{5}}{2\sqrt{13}}$
			^{2}F^0	^{2}F^1	^{2}F^2	^{2}G^0	^{2}G^1	^{2}H
${}^1P$	${}^2D$		$\frac{-\sqrt{7}}{2\sqrt{5}}$	0	0			
${}^3P$			$\frac{3\sqrt{3}}{2\sqrt{35}}$	$\frac{4}{\sqrt{35}}$	0			
${}^1D$			$\frac{1}{\sqrt{14}}$	$\frac{-5\sqrt{3}}{4\sqrt{14}}$	$\frac{\sqrt{3}}{4\sqrt{2}}$	$\frac{1}{\sqrt{3}}$	0	
${}^3D$			$\frac{\sqrt{3}}{\sqrt{14}}$	$\frac{-1}{4\sqrt{14}}$	$\frac{-3}{4\sqrt{2}}$	$\frac{-1}{2}$	$\frac{-\sqrt{5}}{2\sqrt{3}}$	
${}^1F$			$\frac{\sqrt{3}}{\sqrt{10\cdot7}}$	$\frac{-3\sqrt{5}}{4\sqrt{14}}$	$\frac{-\sqrt{5}}{4\sqrt{2}}$	$\frac{-\sqrt{5}}{4\sqrt{3}}$	$\frac{3}{4}$	$\frac{-1}{2}$
${}^3F$			$\frac{3}{\sqrt{10\cdot7}}$	$\frac{-\sqrt{3}}{4\sqrt{10\cdot7}}$	$\frac{\sqrt{15}}{4\sqrt{2}}$	$\frac{-\sqrt{5}}{4}$	$\frac{1}{4\sqrt{3}}$	$\frac{\sqrt{3}}{2}$
			^{4}S	^{4}P	^{4}D^0	^{4}D^1	^{4}F	^{4}G
${}^3P$	${}^2D$			$\frac{3}{2\sqrt{5}}$	$\frac{\sqrt{13}}{2\sqrt{5}}$	0	$\frac{1}{\sqrt{5}}$	
${}^3D$			-1	$\frac{-1}{2\sqrt{3}}$	$\frac{\sqrt{7}}{2\sqrt{13}}$	$\frac{-2\sqrt{2}}{\sqrt{13}}$	$\frac{-1}{\sqrt{2}}$	$\frac{-1}{\sqrt{6}}$
${}^3F$				$\frac{-\sqrt{7}}{\sqrt{15}}$	$\frac{\sqrt{14}}{\sqrt{5\cdot13}}$	$\frac{\sqrt{5}}{\sqrt{13}}$	$\frac{-\sqrt{3}}{\sqrt{10}}$	$\frac{\sqrt{5}}{\sqrt{6}}$

$$
\begin{aligned}
&S^{(1)}_{\rho} = S^{(1)}_{\rho}(1) + S^{(1)}_{\rho}(2) = -i\sqrt{\frac{[\lambda_1]}{2}}\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(01)}_{0\rho} \\
&-i\sqrt{\frac{[\lambda_2]}{2}}\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(01)}_{0\rho}
\end{aligned}
\tag{54}
$$

and also by using relationships

$$
\begin{aligned}
&\left[\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\Lambda_1)} \times \left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\Lambda_2)}\right]^{(\Lambda)}_{M} \\
&= -\sqrt{[\lambda_1, \lambda_2]}\delta(\Lambda_1\Lambda_2, 00) - \sqrt{[\lambda_2]}\left[a^{(\lambda_1)} \times \tilde{a}^{(\lambda_1)}\right]^{(\Lambda)}_{M}\delta(\Lambda_1, 0) \\
&-\sqrt{[\lambda_1]}\left[b^{(\lambda_2)} \times \tilde{b}^{(\lambda_2)}\right]^{(\Lambda)}_{M}\delta(\Lambda_2, 0) - \sum_{\Lambda'\Lambda''}\sqrt{[\Lambda_1, \Lambda_2, \Lambda', \Lambda'']}(-1)^{\Lambda'+\Lambda''-\Lambda} \\
&\times \begin{Bmatrix} \lambda_2 & \lambda_2 & \Lambda_1 \\ \lambda_1 & \lambda_1 & \Lambda_2 \\ \Lambda' & \Lambda'' & \Lambda \end{Bmatrix}\left[\left[\tilde{b}^{(\lambda_2)} \times \tilde{a}^{(\lambda_1)}\right]^{(\Lambda'')} \times \left[b^{(\lambda_2)} \times a^{(\lambda_1)}\right]^{(\Lambda')}\right]^{(\Lambda)}_{M}
\end{aligned}
\tag{55}
$$

and

$$
\begin{aligned}
&\left[\left[\tilde{b}^{(\lambda_2)} \times \tilde{a}^{(\lambda_1)}\right]^{(\Lambda')} \times \left[b^{(\lambda_2)} \times a^{(\lambda_1)}\right]^{(\Lambda')}\right]^{(0)} \\
&= -\sqrt{[\Lambda']} + \sqrt{[\Lambda']}\frac{\widehat{N}_1}{[\lambda_1]} + \sqrt{[\Lambda']}\frac{\widehat{N}_2}{[\lambda_2]} \\
&+ \left[\left[b^{(\lambda_2)} \times a^{(\lambda_1)}\right]^{(\Lambda')} \times \left[\tilde{b}^{(\lambda_2)} \times \tilde{a}^{(\lambda_1)}\right]^{(\Lambda')}\right]^{(0)} \quad , \qquad (56)
\end{aligned}
$$

we get that

$$
\begin{aligned}
&\sum_{\alpha_1 L_1 L'} [L_1] \left(C^2 L'0, C^N \alpha_0 L_0 S_0 = \frac{N_1 + N_2}{2} \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0\right) \\
&\times \left(C^2 L'0, C^N \alpha'_0 L_0 S_0 = \frac{N_1 + N_2}{2} \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0\right) \\
&= \delta(\alpha_0, \alpha'_0)[L_0]\frac{[\lambda_1, \lambda_2] - [\lambda_2]N_1 - [\lambda_1]N_2}{4(N_1+1)(N_2+1)} \ , \qquad (57)
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{\alpha_1 L_1 S_1 L'} [L_1, S_1] \left(C^2 L'1, C^N \alpha_0 L_0 S_0 = \frac{N_1 + N_2}{2} \parallel C^{N+2} \alpha_1 L_1 S_1\right) \\
&\times \left(C^2 L'1, C^N \alpha'_0 L_0 S_0 = \frac{N_1 + N_2}{2} \parallel C^{N+2} \alpha_1 L_1 S_1\right) \qquad (58) \\
&= \delta(\alpha_0, \alpha'_0)[L_0]\frac{(N_1+N_2+1)(4N_1N_2 + 3[\lambda_1, \lambda_2] - 3[\lambda_2]N_1 - 3[\lambda_1]N_2)}{4(N_1+1)(N_2+1)} \ ;
\end{aligned}
$$

if $[\lambda_1] - N_1 = [\lambda_2] - N_2$, then

$$
\begin{aligned}
&\sum_{\alpha_1 L_1 L'} [L_1] \left[\frac{2S_0 - 1}{S_0(2S_0+1)} \left(C^2 L'1, C^N \alpha_0 L_0 S_0 \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0 - 1\right)\right. \\
&\times \left(C^2 L'1, C^N \alpha'_0 L_0 S_0 \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0 - 1\right) \\
&+ \frac{1}{S_0(2S_0+1)} \left(C^2 L'1, C^N \alpha_0 L_0 S_0 \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0\right) \\
&\times \left(C^2 L'1, C^N \alpha'_0 L_0 S_0 \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0\right) \\
&- \frac{2S_0 + 3}{(S_0+1)(2S_0+1)} \left(C^2 L'1, C^N \alpha_0 L_0 S_0 \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0 + 1\right) \\
&\left.\times \left(C^2 L'1, C^N \alpha'_0 L_0 S_0 \parallel C^{N+2} \alpha_1 L_1 S_1 = S_0 + 1\right)\right] \\
&= \delta(\alpha_0, \alpha'_0)(-1)^{2S_0}[L_0]\frac{[\lambda_2] - N_2}{(N_1+1)(N_2+1)} \ , \qquad (59)
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{\alpha_1 L_1 L'} [L_1] \left[\sqrt{S_0} \left(C^2 L'1, C^N \alpha_0 L_0 S_0 \parallel C^{N+2} \alpha_1 L_1 S_0\right)\right. \\
&\times \left(C^2 L'1, C^N \alpha'_0 L_0 S_0 + 1 \parallel C^{N+2} \alpha_1 L_1 S_0\right)
\end{aligned}
$$

$$
\begin{aligned}
&+\sqrt{S_0+2}\left(C^2L'1, C^N\alpha_0L_0S_0 \,\|\, C^{N+2}\alpha_1L_1S_0+1\right)\\
&\times\left(C^2L'1, C^N\alpha_0'L_0S_0+1 \,\|\, C^{N+2}\alpha_1L_1S_0+1\right)\Big] = 0\ ;
\end{aligned}
\tag{60}
$$

if $N_1 = N_2$, then

$$
\begin{aligned}
&\sum_{\alpha_0L_0L'}\Big[(S_1+1)\left(C^2L'1, C^N\alpha_0L_0S_0=S_1-1 \,\|\, C^{N+2}\alpha_1L_1S_1\right)\\
&\times\left(C^2L'1, C^N\alpha_0L_0S_0=S_1-1 \,\|\, C^{N+2}\alpha_1'L_1S_1\right)\\
&+\left(C^2L'1, C^N\alpha_0L_0S_0=S_1 \,\|\, C^{N+2}\alpha_1L_1S_1\right)\\
&\times\left(C^2L'1, C^N\alpha_0L_0S_0=S_1 \,\|\, C^{N+2}\alpha_1'L_1S_1\right)\\
&-S_1\left(C^2L'1, C^N\alpha_0L_0S_0=S_1+1 \,\|\, C^{N+2}\alpha_1L_1S_1\right)\\
&\times\left(C^2L'1, C^N\alpha_0L_0S_0=S_1+1 \,\|\, C^{N+2}\alpha_1'L_1S_1\right)\Big]\\
&=\delta(\alpha_1,\alpha_1')\frac{S_1(S_1+1)}{(N_1+1)}\ ,
\end{aligned}
\tag{61}
$$

$$
\begin{aligned}
&\sum_{\alpha_0L_0L'}\Big[S_1(2S_1+3)\left(C^2L'1, C^N\alpha_0L_0S_0=S_1 \,\|\, C^{N+2}\alpha_1L_1S_1\right)\\
&\times\left(C^2L'1, C^N\alpha_0L_0S_0=S_1 \,\|\, C^{N+2}\alpha_1'L_1S_1+1\right)\\
&+(S_1+2)(2S_1-1)\left(C^2L'1, C^N\alpha_0L_0S_0=S_1+1 \,\|\, C^{N+2}\alpha_1L_1S_1\right)\\
&\times\left(C^2L'1, C^N\alpha_0L_0S_0=S_1+1 \,\|\, C^{N+2}\alpha_1'L_1S_1+1\right)\Big] = 0\ .
\end{aligned}
\tag{62}
$$

First of all, such relationships for the bilinear combinations of CFPs could be useful while determining the expressions of matrix elements of various physical operators. On the other hand, the formulas of summation of CFPs could serve as means of control to test the correctness of the CFPs already tabulated, especially when many different states of a many-electron system occur.

Finally, we would like to make a comment on the method of constructing a basis set of wave functions with the aid of two-shell two-particle CFPs, which is represented by recurrent relationships (45), (50), and (51). The hole representation in any of the shells (or in both) is easy to introduce due to the formalism used, and the relationships obtained do not change in any way and remain valid for any of the representations mentioned of the wave functions and the operators together. By the way, in the hole representation for just one shell, the operator $A_q^{(k)}$ corresponds to the "hopping" of an electron from one shell to another. We stress particularly that in any case while determining the angular parts of matrix elements there is really no need of introducing the quantities other than those already present in (45), (50), and (51).

The method proposed was used in the construction of the basis set atomic wave functions such that the main part of the electrostatic exchange interaction between two different shells is diagonal with respect to the additional quantum numbers α and α'. The matrix element of such an interaction is as follows:

$$\begin{aligned}
&\left\langle \lambda_1^{N_1}\lambda_2^{N_2}\alpha\Lambda M\left|V_{12e}\right|\lambda_1^{N_1}\lambda_2^{N_2}\alpha'\Lambda'M'\right\rangle = 2\cdot\delta(\Lambda M,\Lambda'M') \\
&\times\sum_{\kappa}\frac{(l_1\|\,C^{(\kappa)}\,\|l_2)^2}{[\kappa]}\mathbf{G}_{\kappa}(n_1l_1,n_2l_2)\left\{-\delta(\alpha,\alpha')\frac{[\kappa]}{[\lambda_2]}N_2\right. \\
&+N_1\cdot N_2\cdot\sum_{\alpha''\Lambda''}\left(\lambda_1^1\lambda_2^1(\kappa 0),\lambda_1^{N_1-1}\lambda_2^{N_2-1}\alpha''\Lambda''\right\|\left.\lambda_1^{N_1}\lambda_2^{N_2}\alpha\Lambda\right) \\
&\times\left.\left(\lambda_1^1\lambda_2^1(\kappa 0),\lambda_1^{N_1-1}\lambda_2^{N_2-1}\alpha''\Lambda''\right\|\left.\lambda_1^{N_1}\lambda_2^{N_2}\alpha'\Lambda'\right)\right\}\ ,
\end{aligned}\tag{63}$$

where $\left(\lambda_1^1\lambda_2^1(\kappa 0),\lambda_1^{N_1-1}\lambda_2^{N_2-1}\alpha''\Lambda''\right\|\left.\lambda_1^{N_1}\lambda_2^{N_2}\alpha^{(\prime)}\Lambda^{(\prime)}\right)$ is a new CFP in a hole-particle representation (the first shell, holes; the second, particles; the wave functions in this representation are classified according to the number of hole-particle pairs that they possess). The diagonalization is performed algebraically by a special choice of the numerical values of certain CFPs that are ambiguous otherwise.

Indeed, other parts of interaction instead of the above-mentioned one may be diagonalized this way, provided the interaction is diagonal with respect to Λ quantum numbers.

It is remarkable, however, that the algebraic diagonalization of the main part of the electrostatic exchange interaction between two different shells may yield a basis that is almost diagonal with respect to the full electrostatic interaction. Such are the cases of K and Rb isoelectronic sequences with two open shells np^5nd^2 ($n = 3, 4$), where the weight coefficients of basis functions in simple Hartree-Fock calculations appear to be close to unity. Thus, the algebraically obtained angular coefficients of the new basis could be directly applied in the more rigorous method such as term-dependent Hartree-Fock, which is not the case with the conventional angular coefficients for these sequences.

5. Comments

Although the CR for the wave functions is richer than the SQR in the sense that functions of every permutational symmetry may be represented there, this, unnecessary due to the Pauli principle, richness may lead to complexity, as is the case with the many-shell CFPs. In CFPs expansion formula (26) of the CR, the summation over all the possible configurations of $N - n$ and n electrons for parent terms unavoidably appears, because any attempt to generate a function from a basis where $N-n$- and n-electron configuration functions are mutually nonantisymmetric and those configurations are fixed, leads obviously also to the function of the same symmetry, i.e., the nonantisymmetric one.

Here, we have proved that by the consequent usage of antisymmetrical functions (or equivalently, SQR) one can simplify the many-shell CFPs expansion, getting (31) instead of (26). But this also affects the definition of a CFP. Luckily enough, such reformulation does not affect the numerical values of the single-shell CFPs most commonly used, and change those of the traditional many-shell CFPs by an easily determinable factor, as we have shown in Section 3. The SQR allowed us also to derive the recurrent relationships and other formulas for bilinear combinations of the new CFPs in a rather transparent manner, while in the CR, we know only of an indirect way of obtaining the similar summation rules.

Acknowledgments

We would like to thank Dr. V. Šimonis whose comments and criticisms were useful and whose personal contribution to the present understanding of CFPs problem by one of us (A.B.) is immense. Our former colleague R. Narevičius is thanked for calling our attention to the questions hitherto unclear and for revising some formulae and the table. Also, Professor Z. Rudzikas is particularly thanked for his encouragements and provision of a stimulating atmosphere.

Appendix

Starting from (17) and putting (20) and (21) into it, we get

$$
\begin{aligned}
&\left|\Phi_{ONA}(C^N\alpha\Lambda_0 M_0\{_N x\})\right\rangle = \left(\prod_j N_j!\right)^{-1} \left[C_n^N\right]^{-1/2} \\
&\times \sum_{\{_n x\}=\{x_r \dots x_s\}} (-1)^{P\left(\begin{smallmatrix}1 & \dots & n & n+1 & \dots & N\\ r & \dots & s & t & \dots & u\end{smallmatrix}\right)} \sum_{\{\Lambda_a{}'\}\Lambda'\{\Lambda_a{}''\}\Lambda''\Lambda M} \\
&\longrightarrow \left|\left[\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda'\{_n x\}) \times \Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_M\right\rangle \\
&\times \left\langle\left[\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda'\{_n x\}) \times \Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda''\{_{N-n}x\})\right]^{(\Lambda)}_M\right| \\
&\times \left|\Phi_{ONA}(C^N\alpha\Lambda_0 M_0\{_N x\})\right\rangle \left[C_n^N\right]^{1/2}
\end{aligned}
$$

(here $P\left(\begin{smallmatrix}1 & \dots & n & n+1 & \dots & N\\ r & \dots & s & t & \dots & u\end{smallmatrix}\right)$ stands for the parity of permutation; we decouple the momenta of C^n and C^{N-n} next)

$$
\begin{aligned}
&= \left(\prod_j N_j!\right)^{-1} \left[C_n^N\right]^{-1/2} \sum_{\{_n x\}=\{x_r \dots x_s\}} (-1)^{P\left(\begin{smallmatrix}1 & \dots & n & n+1 & \dots & N\\ r & \dots & s & t & \dots & u\end{smallmatrix}\right)} \\
&\times \sum_{\{\Lambda_a{}'\}\Lambda'\{\Lambda_a{}''\}\Lambda''\Lambda M} \ \sum_{M'M''M_1M_2} \begin{bmatrix} \Lambda' & \Lambda'' & \Lambda \\ M' & M'' & M \end{bmatrix} \begin{bmatrix} \Lambda' & \Lambda'' & \Lambda \\ M_1 & M_2 & M \end{bmatrix} \\
&\times \left|\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda' M'\{_n x\})\right\rangle \left|\Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda'' M''\{_{N-n}x\})\right\rangle \\
&\times \left\langle\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda' M_1\{_n x\})\right| \left\langle\Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda'' M_2\{_{N-n}x\})\right| \\
&\times \left|\Phi_{ONA}(C^N\alpha\Lambda_0 M_0\{_N x\})\right\rangle \left[C_n^N\right]^{1/2}
\end{aligned}
$$

we perform the summation over ΛM and apply the operator (6) in CR for every C^n and C^{N-n} state function:

$$
\begin{aligned}
&= \left(\prod_j N_j!\right)^{-1} \left[C_n^N\right]^{-1/2} \sum_{\{_n x\}=\{x_r \ldots x_s\}} (-1)^{P\left(\begin{smallmatrix} 1 & \ldots & n & n+1 & \ldots & N \\ r & \ldots & s & t & \ldots & u \end{smallmatrix}\right)} \\
&\times \sum_{\{\Lambda_a{}'\}\Lambda'\{\Lambda_a{}''\}\Lambda''\Lambda M} \; \sum_{\alpha_3\Lambda_3 M_3} \left|\Phi_{ONA}(C^n\alpha_3\Lambda_3 M_3\{_n x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^n\alpha_3\Lambda_3 M_3\{_n x\})\right. \left|\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda' M'\{_n x\})\right\rangle \\
&\times \sum_{\alpha_4\Lambda_4 M_4} \left|\Phi_{ONA}(C^{N-n}\alpha_4\Lambda_4 M_4\{_{N-n} x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^{N-n}\alpha_4\Lambda_4 M_4\{_{N-n} x\})\right. \left|\Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda'' M''\{_{N-n} x\})\right\rangle \\
&\times \left[C_n^N\right]^{1/2} \sum_{\alpha_5\Lambda_5 M_5} \left\langle\Phi_{NA}(C^n, \mathrm{A}'\{\Lambda_a{}'\}, \Lambda' M'\{_n x\})\right| \left.\Phi_{ONA}(C^n\alpha_5\Lambda_5 M_5\{_n x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^n\alpha_5\Lambda_5 M_5\{_n x\})\right| \\
&\times \sum_{\alpha_6\Lambda_6 M_6} \left\langle\Phi_{NA}(C^{N-n}, \mathrm{A}''\{\Lambda_a{}''\}, \Lambda'' M''\{_{N-n} x\})\right| \left.\Phi_{ONA}(C^{N-n}\alpha_6\Lambda_6 M_6\{_{N-n} x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^{N-n}\alpha_6\Lambda_6 M_6\{_{N-n} x\})\right| \\
&\times \left|\Phi_{ONA}(C^N\alpha\Lambda_0 M_0\{_N x\})\right\rangle
\end{aligned}
$$

we apply the reverse of (17) for C^n and C^{N-n} states, then:

$$
\begin{aligned}
&= \left(\prod_j C_{n_j}^{N_j}\right)^{-1} \left[C_n^N\right]^{-1/2} \sum_{\{_n x\}=\{x_r \ldots x_s\}} (-1)^{P\left(\begin{smallmatrix} 1 & \ldots & n & n+1 & \ldots & N \\ r & \ldots & s & t & \ldots & u \end{smallmatrix}\right)} \\
&\times \left[C_n^N\right]^{1/2} \sum_{\alpha_3\Lambda_3 M_3} \; \sum_{\alpha_5\Lambda_5 M_5} \left|\Phi_{ONA}(C^n\alpha_3\Lambda_3 M_3\{_n x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^n\alpha_3\Lambda_3 M_3\{_n x\})\right| \left.\Phi_{ONA}(C^n\alpha_5\Lambda_5 M_5\{_n x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^n\alpha_5\Lambda_5 M_5\{_n x\})\right| \\
&\times \sum_{\alpha_4\Lambda_4 M_4} \; \sum_{\alpha_6\Lambda_6 M_6} \left|\Phi_{ONA}(C^{N-n}\alpha_4\Lambda_4 M_4\{_{N-n} x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^{N-n}\alpha_4\Lambda_4 M_4\{_{N-n} x\})\right| \left.\Phi_{ONA}(C^{N-n}\alpha_6\Lambda_6 M_6\{_{N-n} x\})\right\rangle \\
&\times \left\langle\Phi_{ONA}(C^{N-n}\alpha_6\Lambda_6 M_6\{_{N-n} x\})\right| \\
&\times \left|\Phi_{ONA}(C^N\alpha\Lambda_0 M_0\{_N x\})\right\rangle
\end{aligned}
$$

and perform the summations over $\alpha_5\Lambda_5 M_5$ and $\alpha_6\Lambda_6 M_6$:

$$
\begin{aligned}
&= \left(\prod_j C_{n_j}^{N_j}\right)^{-1} \left[C_n^N\right]^{-1/2} \sum_{\{_n x\}=\{x_r \ldots x_s\}} (-1)^{P\left(\begin{smallmatrix} 1 & \ldots & n & n+1 & \ldots & N \\ r & \ldots & s & t & \ldots & u \end{smallmatrix}\right)} \\
&\times \left[C_n^N\right]^{1/2} \sum_{\alpha_3\Lambda_3 M_3} \; \sum_{\alpha_4\Lambda_4 M_4} \left|\Phi_{ONA}(C^n\alpha_3\Lambda_3 M_3\{_n x\})\right\rangle \\
&\times \left|\Phi_{ONA}(C^{N-n}\alpha_4\Lambda_4 M_4\{_{N-n} x\})\right\rangle \left\langle\Phi_{ONA}(C^{N-n}\alpha_4\Lambda_4 M_4\{_{N-n} x\})\right|
\end{aligned}
$$

$$\times \langle \Phi_{ONA}(C^n \alpha_3 \Lambda_3 M_3 \{_n x\})|$$
$$\times \left| \Phi_{ONA}(C^N \alpha \Lambda_0 M_0 \{_N x\}) \right\rangle$$

after replacements $\alpha_3\Lambda_3 M_3 \longrightarrow \alpha'\Lambda' M'$, $\alpha_4\Lambda_4 M_4 \longrightarrow \alpha''\Lambda'' M''$ and coupling of the momenta of C^n and C^{N-n} again:

$$= \left(\prod_j C_{n_j}^{N_j} \right)^{-1} \left[C_n^N \right]^{-1/2} \sum_{\{_n x\} = \{x_r \dots x_s\}} (-1)^{P\left(\begin{smallmatrix} 1 & \dots & n & n+1 & \dots & N \\ r & \dots & s & t & \dots & u \end{smallmatrix}\right)}$$
$$\times \left[C_n^N \right]^{1/2} \sum_{\alpha'\Lambda' M'} \sum_{\alpha''\Lambda'' M''} \sum_{\Lambda_1 M_1} \sum_{\Lambda_2 M_2} \begin{bmatrix} \Lambda' & \Lambda'' & \Lambda_1 \\ M' & M'' & M_1 \end{bmatrix} \begin{bmatrix} \Lambda' & \Lambda'' & \Lambda_2 \\ M' & M'' & M_2 \end{bmatrix}$$
$$\times \left| \left[\Phi_{ONA}(C^n \alpha' \Lambda' \{_n x\}) \times \Phi_{ONA}(C^{N-n} \alpha'' \Lambda'' \{_{N-n} x\}) \right]^{(\Lambda_1)}_{M_1} \right\rangle$$
$$\times \left\langle \left[\Phi_{ONA}(C^n \alpha' \Lambda' \{_n x\}) \times \Phi_{ONA}(C^{N-n} \alpha'' \Lambda'' \{_{N-n} x\}) \right]^{(\Lambda_2)}_{M_2} \right|$$
$$\times \left| \Phi_{ONA}(C^N \alpha \Lambda_0 M_0 \{_N x\}) \right\rangle$$

we perform the summation over $M'M''$ now:

$$= \left(\prod_j C_{n_j}^{N_j} \right)^{-1} \left[C_n^N \right]^{-1/2} \sum_{\{_n x\} = \{x_r \dots x_s\}} (-1)^{P\left(\begin{smallmatrix} 1 & \dots & n & n+1 & \dots & N \\ r & \dots & s & t & \dots & u \end{smallmatrix}\right)}$$
$$\times \left[C_n^N \right]^{1/2} \sum_{\alpha'\Lambda'} \sum_{\alpha''\Lambda''} \sum_{\Lambda_1 M_1} \sum_{\Lambda_2 M_2} \delta(\Lambda_1 M_1, \Lambda_2 M_2)$$
$$\times \left| \left[\Phi_{ONA}(C^n \alpha' \Lambda' \{_n x\}) \times \Phi_{ONA}(C^{N-n} \alpha'' \Lambda'' \{_{N-n} x\}) \right]^{(\Lambda_1)}_{M_1} \right\rangle$$
$$\times \left\langle \left[\Phi_{ONA}(C^n \alpha' \Lambda' \{_n x\}) \times \Phi_{ONA}(C^{N-n} \alpha'' \Lambda'' \{_{N-n} x\}) \right]^{(\Lambda_2)}_{M_2} \right|$$
$$\times \left| \Phi_{ONA}(C^N \alpha \Lambda_0 M_0 \{_N x\}) \right\rangle$$

and, finally, after a trivial summation over $\Lambda_2 M_2$ and a replacement $\Lambda_1 M_1 \longrightarrow \Lambda M$:

$$= \left(\prod_j C_{n_j}^{N_j} \right)^{-1} \sum_{\alpha'\Lambda'\alpha''\Lambda''\Lambda M} \left| \Phi_{NA}(C^n \alpha' \Lambda', C^{N-n} \alpha'' \Lambda'', \Lambda M \{_N x\}) \right\rangle$$
$$\times \left\langle \Phi_{NA}(C^n \alpha' \Lambda', C^{N-n} \alpha'' \Lambda'', \Lambda M \{_N x\}) \left| \Phi_{ONA}(C^N \alpha \Lambda_0 M_0 \{_N x\}) \right\rangle \right. ,$$

where, similarly as in (20) and (21)

$$\left| \Phi_{NA}(C^n \alpha' \Lambda', C^{N-n} \alpha'' \Lambda'', \Lambda M \{_N x\}) \right\rangle$$
$$\equiv \widehat{\mathbf{A}} \left| \left[\Phi_{ONA}(C^n \alpha' \Lambda' \{_n x\}) \times \Phi_{ONA}(C^{N-n} \alpha'' \Lambda'' \{_{N-n} x\}) \right]^{(\Lambda)}_{M} \right\rangle ,$$

and then

$$\left\langle \Phi_{NA}(C^n\alpha'\Lambda', C^{N-n}\alpha''\Lambda'', \Lambda M\{_N x\}) \,\middle|\, \Phi_{ONA}(C^N\alpha\Lambda_0 M_0\{_N x\}) \right\rangle$$
$$= \left[C_n^N\right]^{1/2} \left\langle \left[\Phi_{ONA}(C^n\alpha'\Lambda'\{_n x\}) \times \Phi_{ONA}(C^{N-n}\alpha''\Lambda''\{_{N-n} x\})\right]^{(\Lambda_2)}_{M_2} \right|$$
$$\times \left| \Phi_{ONA}(C^N\alpha\Lambda_0 M_0\{_N x\}) \right\rangle \ .$$

Bibliography

[1] B.R.Judd, *Second Quantization and Atomic Spectroscopy* (Johns Hopkins Press, Baltimore, 1967).

[2] R.D.Lawson and M.H.Macfarlane, Nucl. Phys. **66**, 80 (1965).

[3] J.M.Kaniauskas and Z.B.Rudzikas, J. Phys. B **13**, 3521 (1980).

[4] J.M.Kaniauskas and Z.B.Rudzikas, *Quasispin and Isospin in Atomic Theory* (Mokslas, Vilnius, 1984) (in Russian).

[5] P.A.M.Dirac, *The Principles of Quantum Mechanics* 4th ed. (Clarendon Press, Oxford, 1958).

[6] A.P.Jucys and A.A.Bandzaitis, *Theory of Angular Momentum in Quantum Mechanics* (Mokslas, Vilnius, 1977) (in Russian).

[7] S.Meshkov, Phys. Rev. **99**, 871 (1953); I.Levinson, Trudy Akademii Nauk Litovskoi SSR Ser. B, **4**, 17 (1957) (in Russian).

[8] U.Fano, Phys. Rev. **140**, A67 (1965).

[9] G.Racah, Phys. Rev. **62**, 438 (1942).

[10] J.N.Ginocchio, Nucl. Phys. **74**, 321 (1965); K.T.Hecht, Phys. Rev. **139** (4B) 794 (1965).

[11] I.S.Kichkin and Z.B.Rudzikas, Litovskii Fizicheskii Sbornik **11**, 743 (1971) (in Russian).

[12] A.Bernotas, V.Šimonis and Z.Rudzikas, Soviet Phys. Coll. **27**(6) 1 (1987); V.Šimonis, A.Bernotas, and Z.Rudzikas, Soviet Phys. Coll. **27**(6) 11 (1987) (Available from Allerton Press).

[13] P.J.Redmond, Proc. R. Soc. A **222**, 84 (1954).

[14] B.R.Judd, *Topics in Atomic Theory* (University of Canterbury, New Zealand, 1969).

[15] A.Bernotas, J.Kaniauskas, and Z.Rudzikas, Lithuanian Phys. J. (formerly Soviet Phys. Coll.) **29**(4) 30 (1989) (Available from Allerton Press).

[16] A.P.Jucys and A.J.Savukynas, *Mathematical Foundations of the Atomic Theory* (Mintis, Vilnius, 1973) (in Russian).

[17] V.Šimonis, A.Bernotas, Lithuanian Physics Journal (formerly Soviet Phys. Coll.) **29**(5) 1 (1989) (Available from Allerton Press).

Received May 15, 1993
Accepted for publication September 21, 1993