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Algebraic development of many-body perturbation theory in theoretical atomic spectroscopy

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1 Introduction

In atomic spectroscopy, a powerful mathematical tool for theoretical study of electron correlation effects as well as the atomic parity violation, ultra-cold collisions and much greater of many-electron problems, is based on irreducible tensor formalisms and, consequently, on symmetry principles, simplifying various expressions, thus considerably reducing amount of further on theoretical calculations of desirable physical quantities. The mathematical formulation of irreducible tensor operators gained appropriate grade in modern physics due to well-developed theories of group representations. Namely, in the manner of representations, the group operations are accomplished on vector spaces over real, complex, etc. fields, defining vector-valued functions and their behaviour under various transformations. Therein the fundamental connection between measurable physical quantities and abstract operators on Hilbert space—particularly those transforming under irreducible representations—is realised through the bilinear functionals which ascertain, in general, the mapping from the Kronecker product of vector spaces into some given unitary or Euclidean vector space. In physical applications, these bilinear forms, usually called the matrix elements on given basis, are selected to be self-adjoint.

The physical processes and various spectroscopic magnitudes, such as, for example, electron transition probability, energy width of level or lifetime of state of level, electron interactions and many more, are uniformly estimated by the corresponding operator matrix elements on the basis of eigenfunctions of the Hamiltonian which characterises the studied process. To this day, the most widely used method to construct the basis functions is based on the atomic shell model suggested by N. Bohr [1] and later adapted to the nuclear shell model that was first proposed by M. G. Mayer and J. H. D. Jensen [2–4]. In this model, electron states in atom are characterised by the nonnegative integers which in their turn form the set of quantum numbers describing the Hamiltonian of a local or stationary system. For the most part, the nonnegative integers that describe the dynamics of such system simply mark off the irreducible group representations if the group operators commute with a Hamiltonian. Particularly, in the atomic central-field approximation, the Hamiltonian is invariant under reflection and rotation in $\mathbf{R}^3$, thus the eigenstate of such Hamiltonian is characterised by the parity Π of configuration and by the $\mathrm{SO}(3)$–irreducible representation L, also known as the angular momentum. Within the framework of the last approximation, the atomic Hamiltonian may be constructed by making it the $\mathrm{SU}(2)$–invariant, since $\mathrm{SU}(2)$ is a double covering group of $\mathrm{SO}(3)$. Then the eigenstate is characterised additionally by the $\mathrm{SU}(2)$–irreducible representation J, also known as the total angular momentum. The theory of angular momentum was first offered by E. U. Condon, G. H. Shortley [5] and later much more extended by E. Wigner, G. Racah [6–9] and A. P. Jucys et. al. [10–12]. Although the methods to reduce the Kronecker products of the irreducible representations which label, particularly, the irreducible tensor operators, are extensively developed by many researchers until now [13–17], still there are a lot of predicaments to choose a convenient reduction scheme which ought to diminish the time resources for a large scale of theoretical calculations. The problems to prepare the effective techniques of reduction are dominant especially in the studies of open-shell atoms, when dealing with the physical as well as the effective none scalar irreducible tensor operators and their matrix elements on the basis of complex configuration functions.

A total eigenfunction of atomic stationary Hamiltonian is built up beyond the central-field approach and it is, by the origin, the major object of the many-body theories. Unfortunately, the exact eigenstates can not be found, thus the final results that characterise the dynamics of such complex system are not yet possible. From the mathematical point of view, the eigenstates of Hamiltonian form some linear space. If the spectrum of Hamiltonian is described by discrete levels, then the eigenstates characterised by the nonnegative integers form a separable Hilbert space; otherwise, the linear space is, in general, non-separable. Through ignorance of the structure of exact eigenstates, there are formed the linear combinations of the basis functions that are usually far from the exact picture. The basis functions are selected to be the eigenstates of the central-field Hamiltonian. This yields various versions of the multi-configuration Hartree–Fock (MCHF) approach based on the variation of the energy functional with respect to single-electron wave functions. In this approach, a huge number of admixed configurations together with high order of energy matrices need to be taken into account [18–20]. By the mathematical formu-

lation, the multi-configuration function is considered as the superposition of the configuration state functions (CSF), thus the present approximation is confined to be in operation on a *single* many-particle Hilbert space. Contrary to this model, there exists another extremely different method to build the exact eigenfunction of many-particle system. Of special interest is the atomic many-body perturbation theory (MBPT) that accounts for a *variable* number of many-particle Hilbert spaces simultaneously. Therefore, the latter approximation is in operation on a Fock space.

The MBPT—due to its versatility—is widespread until nowadays not only in atomic physics. Namely, the main idea of present approximation has been appropriated, as it became usual, from the theory of nucleus followed by the works of K. A. Brueckner and J. Goldstone [21–23], and afterwards adapted to atomic physics and quantum chemistry [24–33]. In most general case, the eigenfunction of many-particle Hamiltonian is generated by the exponential ansatz which acts on the unit vector of the entire Hilbert space, also known as the genuine vacuum. In perturbation theory (PT), the exponential ansatz is frequently defined to obey the form of the so-called wave operator acting on a reference function or else the physical vacuum. Such formulation is followed by the Fock space theory, studied in detail by W. Kutzelnigg [31] and by the particle-hole picture, recently exploited by many authors in modern MBPT [34–38]. For the closed-shell atoms, the reference function simply denotes a single Slater determinant which represents an eigenfunction of the central-field Hamiltonian. Attempts to construct the reference function for the open-shell atoms lead to a much more complicated task. By traditional procedure, the entire Hilbert space is partitioned into two subspaces, where the first one is spanned by the multi-configuration state functions associated with the eigenvalues of the central-field Hamiltonian, and the second one is formed from the functions which are absent in the first subspace. The reason for such partitioning is that for open-shell atoms the energy levels are degenerate and the full set of reference functions is not always determined initially. Therefore the number of selected functions denotes the dimension of a subspace usually called the model space [39]. A universal algorithm to form the model space in open-shell MBPT is yet impossible and the problem under consideration still insists on further studies.

A significant advantage of the MBPT is that the exact eigenvalues of atomic Hamiltonian are obtained even without knowing the exact eigenfunctions. The number of solutions for energies is made dependent on a dimension of model space. To solve this task, the eigenvalue equation is addressed to finding the operator which acts on chosen model space. The form of the latter operator, called the effective Hamiltonian [34], is closely related to the form of wave operator. Usually, there are distinguished Hilbert-space and Fock-space approaches, in order to specify this operator. In the Hilbert-space approach, the model space is chosen to include a fixed number of electrons. Then the wave operator is determined by eigenvalue equation of atomic Hamiltonian for a single many-particle Hilbert space only. In this sense, it is similar to the multi-configuration approach. In the Fock-space approach, the wave operator is represented equally on all many-particle Hilbert spaces which are formed by the functions with a variable number of valence electrons of open-shell atom. By the mathematical formulation, the Fock-space approximation is based on the occupation-number representation. Consequently, this treatment suggests the possibility of simultaneously taking into account for the effects that are conditioned by the variable number of particles. Starting from this point of view, several variations to construct the effective interaction operator on a model space are separated resulting in different versions of the PT. Nevertheless, a general idea embodied in all perturbation theories states that the Hamiltonian of many-particle system splits up into the unperturbed Hamiltonian and the perturbation which characterises the inhomogeneity of system. In atomic physics, the unperturbed Hamiltonian stands for a usual central-field Hamiltonian. The major difficulties arise due to the perturbation. In various versions of PT, the techniques to account for the perturbation differ. The Rayleigh–Schrödinger (RS) and coupled-cluster (CC) theories combined with the second quantisation representation (SQR) are the most common approaches used in theoretical atomic physics. The perturbation series is built by using the Wick's theorem [40] which makes it possible to evaluate the products of the Fock space operators. The number of these products grows rapidly as the order of perturbation increases. For this reason, the RSPT is applied to a finite-order perturbation, when constructing the many-electron wave function of a fixed order m, starting from $m = 0$ step by step [36, 37, 41]. In CC theory, the initially

given exponential ansatz is represented, in general, as an infinite sum of Taylor series. The total eigenfunction is then expressed by the sum of all-order n–particle ($n = 0, 1, 2, \ldots$) functions, denoting zero-, single-, double-, etc. excitations [35,42]. However, in practical applications, the sum of terms is also finite. To this day, the progressive attempts to evaluate the terms of atomic PT by using the computer algebra systems have been reported by a number of authors [43–45].

One more problem ordinary to open-shell MBPT is to handle the generated terms of PT. In addition to a large number of terms from given scale, each term has to be separately worked up for a convenient usage, in order to calculate the energy corrections efficiently. This is done by using the angular momentum theory (AMT) combined with the tensor formalism. In atomic spectroscopy, the theoretical foundation of tensor operator technique has been built by Judd et. al. [46–49] and later extended by Rudzikas et. al. [50–55]. In the occupation-number representation, the terms of PT are reduced to the effective n–particle operators. In most cases, authors account for the zeroth, single and double ($n = 0, 1, 2$) particle-hole excitations. First of all, this is due to their biggest part of contribution to the correlation energy. Secondly, it is determined by the complexity of structure of the irreducible tensor operators that act on more than four open shells ($n > 2$). For example, in his study of the wave functions for atomic beryllium [56], Bunge calculated that the contribution of double excitations to the correlation energy for the Be atom represented about 95%, while the triple excitations made approximately 1% of the contribution. On the other hand, in modern physics, the high-level accuracy measured bellow 0.1% is desirable especially in the studies of atomic parity violation [57] or when accounting for radiative corrections of hyperfine splittings in alkali metals or highly charged ions [58]. Such level of accuracy is obtained when the triple excitations are involved in the series of the PT, as demonstrated by Porsev et. al. [42]. This indicates that the mathematical techniques applied to the reduction of the tensor products of the Fock space operators still are urgent and inevitable.

1.1 The main goals of present work

1. To work out the versatile disposition methods and forms pertinent to the tensor products of the irreducible tensor operators which represent either physical or effective interactions considered in the atomic open-shell many-body perturbation theory.

2. To create a symbolic computer algebra package that handles complex algebraic manipulations used in modern theoretical atomic spectroscopy.

3. Making use of the symbolic computer algebra and mathematical techniques, to explore the terms of atomic open-shell many-body perturbation theory in a Fock-space approach, paying special attention to the construction of a model space and the development of angular reduction of terms that fit a fixed-order perturbation. Meanwhile, to elaborate the reduction scheme suitable for an arbitrary order perturbation or a coupled-cluster expansion.

1.2 The main tasks

1. To find regularities responsible for the behaviour of operators on various subspaces of the entire Fock space. To study the properties and consequential causes made dependent on the condition that a set of eigenvalues of Hamiltonian on the infinite-dimensional Hilbert space contains a subset of eigenvalues of Hamiltonian projected onto the finite-dimensional subspace.

2. To classify the totally antisymmetric tensors determined by the Fock space operator string of any length. To determine the transfer attributes of irreducible tensor operators associated to distinct angular reduction schemes.

3. To generate the terms of the second-order wave operator and the third-order effective Hamiltonian on the constructed finite-dimensional subspace by using a produced symbolic computer algebra package. To develop the approach of many-particle effective matrix elements so that the projection-independent parts could be easy to vary remaining steady the tensor structure of expansion terms.

1.3 The scientific novelty

1. Opposed to the usual Slater-type orbitals, the $\mathrm{SU}(2)$–irreducible matrix representations have been demonstrated to be a convenient basis for the calculation of matrix elements of atomic quantities. A prominent part of such type of computations is in debt to the newly found $\mathrm{SO}(3)$–irreducible tensor operators.

2. Bearing in mind that the theoretical interpretation concerned with the model space in open-shell many-body perturbation theory is poorly defined so far, attempts to give rise to more clarity have been initiated. The key result which causes to diminish the number of expansion terms is that only a fixed number of types of the Hilbert space operators with respect to the single-electron states attach the non-zero effective operators on the constructed model space.

3. The algorithm to classify the operators observed in the applications of effective operator approach to the atomic open-shell many-body perturbation theory has been produced. The classification of three-particle effective operators that act on 2, 3, 4, 5, 6 electron shells of atom has been performed expressly. As a result, the calculation of matrix elements of three-particle operators associated to any angular reduction scheme becomes easily performed.

4. The angular reduction of terms of the third-order effective Hamiltonian on the constructed model space has been performed in extremely different way than it has been done so far. To compare with a usual diagrammatic formulation of atomic perturbation theory, the principal advantages of such technique are: (i) the ability to vary the amplitudes of electron excitation suitable for special cases of interest – the tensor structure is free from the change; (ii) the ability to enclose a number of Goldstone diagrams by the sole tensor structure. As a result, the problem of evaluation of each separate diagram is eliminated.

1.4 Statements to be defended

1. The integrals over S^2 of the $\mathrm{SO}(3)$–irreducible matrix representation parametrised by the coordinates of $S^2 \times S^2$ constitute a set of components of $\mathrm{SO}(3)$–irreducible tensor operator.

2. There exists a finite-dimensional subspace of infinite-dimensional many-electron Hilbert space such that the non-zero terms of effective atomic Hamiltonian on the subspace are generated by a maximum of eight types of the n–body parts of wave operator with respect to the single-electron states for all nonnegative integers n.

3. The method developed by making use of the S_ℓ–irreducible representations, the tuples and the commutative diagrams of maps associating distinct angular reduction schemes makes it possible to classify the angular reduction schemes of antisymmetric tensors of any length in an easy to use form that stipulates an efficiency of calculation of matrix elements of complex irreducible tensor operators.

4. The restriction of many-electron Hilbert space the wave operator acts on to its $\mathrm{SU}(2)$–irreducible subspaces guarantees the ability to enclose a number of Goldstone diagrams by the sole tensor structure so that the amplitudes of electron excitation are easy to vary depending on the specific cases of interest, but the tensor structure of expansion terms is fixed.

1.5 List of publications

1. R. Juršėnas and G. Merkelis, *Coupling schemes for two-particle operator used in atomic calculations*, Lithuanian J. Phys. **47**, no. 3, 255 (2007)

2. R. Juršėnas, G. Merkelis, *Coupled tensorial form for atomic relativistic two-particle operator given in second quantization representation*, Cent. Eur. J. Phys. **8**, no. 3, 480 (2010)

3. R. Juršėnas and G. Merkelis, *Coupled tensorial forms of the second-order effective Hamiltonian for open-subshell atoms in jj-coupling*, At. Data Nucl. Data Tables (2010), doi:10.1016/j.adt.2010.08.001

4. R. Juršėnas and G. Merkelis, *Application of symbolic programming for atomic many-body theory*, Materials Physics and Mechanics **9**, no. 1, 42 (2010)

5. R. Juršėnas, G. Merkelis, *The transformation of irreducible tensor operators under spherical functions*, Int. J. Theor. Phys. **49**, no. 9, 2230 (2010)

6. R. Juršėnas, G. Merkelis, *Irreducible tensor form of three-particle operator for open-shell atoms*, Cent. Eur. J. Phys. (2010), doi: 10.2478/s11534-010-0082-0

7. R. Juršėnas and G. Merkelis, *Development of algebraic techniques for the atomic open-shell MBPT (3)*, to appear in J. Math. Phys. (2010)

1.6 List of abstracts

1. R. Juršėnas, G. Merkelis, *Coupling schemes for two-particle operator used in atomic calculations*, 37th Lithuanian National Physics Conference, Vilnius, 2007, Abstracts, p. 219

2. R. Juršėnas, *Coupled tensorial forms of atomic two-particle operator*, 40th EGAS Conference, Graz, 2008, Abstracts, p. 45

3. R. Juršėnas, G. Merkelis, *Coupled tensorial forms of the second-order effective Hamiltonian for open-subshell atoms in jj-coupling*, 38th Lithuanian National Physics Conference, Vilnius, 2009, p. 229

4. R. Juršėnas, G. Merkelis, *Symbolic programming applications for atomic many-body theory*, 13th International Workshop on New Approaches to High Tech: Nano Design, Technology, Computer Simulations, Vilnius, 2009, Abstracts, p. 22

5. R. Juršėnas, G. Merkelis, *The MBPT study of electron correlation effects in open-shell atoms using symbolic programming language Mathematica*, 41st EGAS Conference, Gdansk, 2009, Abstracts, p. 102

6. R. Juršėnas and G. Merkelis, *Algebraic exploration of the third-order MBPT*, Conference on Computational Physics, Trondheim, 2010, Abstracts, p. 213

7. R. Juršėnas, G. Merkelis, *The transformation of irreducible tensor operators under the spherical functions*, ECAMP10, Salamanca, 2010, Abstracts, p. 87

8. R. Juršėnas, G. Merkelis, *The generation and analysis of expansion terms in the atomic stationary perturbation theory*, ICAMDATA 7, Vilnius, 2010, Abstracts, p. 86

2 Partitioning of function space and basis transformation properties

Two mathematical notions exploited in atomic physics are discussed: the first and second quantisation representations. In the first representation, the basis transformation properties—fixed to a convenient choice—are developed. In the second representation, many-electron systems with variable particle number are studied—concentrating on partitioning techniques of function space—to improve the efficiency of effective operator approach.

The key results are the composed $\mathrm{SO}(3)$–irreducible tensor operators, the technique—based on coordinate transformations—to calculate the integrals of many-electron angular parts, the Fock space formulation of the generalised Bloch equation, the theorem that determines non-zero effective operators on the bounded subspace of infinite-dimensional many-electron Hilbert space.

This section is organised as follows. In Sec. 2.1, the widespread methods to construct a total wave function of atomic many-body system are briefly presented. Sec. 2.2 studies the $\mathrm{SU}(2)$–irreducible matrix representations and their parametrisations. The inspiration for the parametrisation of matrix representation in a specified form came from the properties characteristic to irreducible tensor operators, usually studied in theoretical atomic spectroscopy. Sec. 2.2.2 demonstrates the application of method based on the properties of founded new set of irreducible tensor operators. In Sec. 2.3, the second quantised formalism applied to the atomic systems is developed. The advantages of perturbative methods to compare with the variational approach are revealed. The effective operator approach, as a direct consequence of the so-called partitioning technique (Sec. 2.3.1), is developed in Sec. 2.3.2.

2.1 The integrals of motion

The quantum mechanical interpretation of atomic many-body system is found to be closely related to the construction of Hamiltonian H. In a time-independent approach, this Hamiltonian corresponds to the total energy E of system. To find E, the eigenvalue equation of H must be solved. The eigenfunction Ψ of H depends on the symmetries that are hidden in the many-body system Hamiltonian. The group-theoretic formulation of the problem is to find the group G such that the operators $\widehat{g} \in G$ commute with H. That is, if $[H, \widehat{g}] = 0$, then Ψ is characterised by the irreducible representations (or «irrep» for short) of G. A well-known example is the Bohr or central-field Hamiltonian $\widetilde{H}_0 = T + U_C$ of the N–electron atom, where T represents the kinetic energy of electrons and U_C denotes the Coulomb (electron-nucleus) potential. This Hamiltonian is invariant under the rotation group $G = \mathrm{SO}(3)$ with $\widehat{g} \in \{\widehat{L}_1, \widehat{L}_2, \widehat{L}_3\}$ being the infinitesimal operator or else the angular momentum operator. Consequently, the eigenfunctions Ψ are characterised by the irreducible representations $L = 0, 1, \ldots$ of $\mathrm{SO}(3)$ and by the indices $M = -L, -L+1, \ldots, L-1, L$ that mark off the eigenstates of $\widehat{L}_i$ $(i = 1, 2, 3)$. In this case, we write $\Psi \equiv \Psi(\Gamma LM|\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \equiv \Psi(\Gamma LM)$, where $\boldsymbol{x}_\xi \equiv r_\xi \widehat{x}_\xi$ denotes the radial r_ξ and spherical $\widehat{x}_\xi \equiv \theta_\xi \varphi_\xi$ coordinates of the ξth electron. The quantity Γ denotes the rest of numbers that append the other, if any, symmetry properties involved in $\widetilde{H}_0$. Particularly, the Bohr Hamiltonian $\widetilde{H}_0$ is also invariant under the reflection characterised by the parity Π. Thus $\widetilde{H}_0$ implicates the symmetry group $\mathrm{O}(3)$.

The infinitesimal operators $\widehat{L}_i$ form the B_1 Lie algebra (in Cartan's classification) which is isomorphic to the A_1 algebra formed by the generators $\widehat{J}_i$. Besides, it is known [59, Sec. 5.5.2, p. 99] that the angular momentum operator $\widehat{L}_i$ is the sum of two independent A_1 Lie algebras formed by $\widehat{J}_i^{\pm}$. This implies that $\widetilde{H}_0$ is also invariant under $\mathrm{SU}(2)$ operations and thus Ψ may be characterised by the $\mathrm{SU}(2)$–irreducible representation $J = 1/2, 3/2, \ldots$ which particularly characterises the spin-$1/2$ particles (electrons).

Regardless of well-defined symmetries appropriated by $\widetilde{H}_0$, the central-field approximation does not account for the interactions between electrons. In order to do so, the total Hamiltonian H of N–electron system is written as follows

$$H = H_0 + V, \quad H_0 = \widetilde{H}_0 + U. \tag{2.1}$$

The Hamiltonian H_0 pertains to the symmetry properties of $\widetilde{H}_0$ since U represents the central-

field potential which has the meaning of the average Coulomb interaction of electron with the other electrons in atom [34, Sec. 5.4, p. 114]. All electron interactions along with external fields, if such exist, are drawn in the perturbation V. It seems to be obvious that the structure of H is much more complicated than the structure of H_0.

Having defined the Hamiltonian H and assuming that the eigenfunctions $\{\Psi_i\}_{i=1}^{\infty} \equiv X$ form the infinite-dimensional Hilbert space $\mathcal{H}$ with the scalar product $\langle ,\cdot, \rangle_{\mathcal{H}} \colon X \times X \longrightarrow \mathbb{R}$, the energy levels E_i are expressed by $\langle \Psi_i \cdot H\Psi_i \rangle_{\mathcal{H}} \equiv \langle \Psi_i | H | \Psi_i \rangle$. Since the functions Ψ_i are unknown, usually they are expressed by the linear combination of some initially known basis Φ_i. With such definition, the relation reads

$$\Psi(\Gamma_i \Pi_i \Lambda_i M_i) = \sum_{\widetilde{\Gamma}_i} c_{\widetilde{\Gamma}_i \Pi_i \Lambda_i} \Phi(\widetilde{\Gamma}_i \Pi_i \Lambda_i M_i), \quad c_{\widetilde{\Gamma}_i \Pi_i \Lambda_i} \in \mathbb{R}. \tag{2.2}$$

Here $\Lambda_i M_i \equiv L_i S_i M_{L_i} M_{S_i}$ or $\Lambda_i M_i \equiv J_i M_{J_i}$ depend on the symmetry group assuming that the functions Φ_i represent the eigenfunctions of H_0. The real numbers $c_{\widetilde{\Gamma}_i \Pi_i \Lambda_i}$ are found by diagonalizing the matrix of H on the basis Φ_i, where the entries of matrix are

$$H_{\Gamma_i \Gamma_i'} = \delta_{\Pi_i \Pi_i'} \delta_{\Lambda_i \Lambda_i'} \delta_{M_i M_i'} \langle \Gamma_i \Pi_i \Lambda_i M_i | H | \Gamma_i' \Pi_i' \Lambda_i' M_i' \rangle. \tag{2.3}$$

If, particularly, H is the scalar operator, then the $H_{\Gamma_i \Gamma_i'}$ do not depend on M_i.

The solutions Φ_i of central-field equation, the configuration state functions (CSF), are found by making the antisymmetric products or Slater determinants [60, p. 1300] of single-electron functions $R(n_\xi \kappa_\xi | r_\xi) \phi(\lambda_\xi m_\xi | \widehat{x}_\xi)$, characterised by the numbers $\lambda_\xi \equiv l_\xi 1/2$ or $\lambda_\xi \equiv j_\xi$, where $\xi = 1, 2, \ldots, N$, $l_\xi = 0, 1, \ldots$ and $j_\xi = 1/2, 3/2, \ldots$. The quantity κ_ξ depends on the symmetry group. For $G = \mathrm{SO}(3)$, $\kappa_\xi \equiv l_\xi$; for $G = \mathrm{SU}(2)$, $\kappa_\xi \equiv l_\xi j_\xi$, where $l_\xi = 2j_\xi \pm 1$. The functions $\phi(\lambda_\xi m_\xi | \widehat{x}_\xi)$ are transformed by the irreducible unitary matrix representations of $G = \mathrm{SU}(2)$. These representations denote the matrix $D^{\lambda_\xi}(g)$ of dimension $\dim D^{\lambda_\xi}(g) = 2\lambda_\xi + 1$, where $g \in G$. That is,

$$D^{\lambda_\xi \dagger}(g) \phi(\lambda_\xi m_\xi | \widehat{x}_\xi) = \sum_{\widetilde{m}_\xi} D^{\lambda_\xi}_{m_\xi \widetilde{m}_\xi}(g) \phi(\lambda_\xi \widetilde{m}_\xi | \widehat{x}_\xi). \tag{2.4}$$

The explicit form of element $D^{\lambda_\xi}_{m_\xi \widetilde{m}_\xi}(g)$ depends on the parameters g and basis. The parametrisation of $D^{\lambda_\xi}_{m_\xi \widetilde{m}_\xi}(\Omega)$ by the Euler angles $\Omega = (\Phi, \Theta, \Psi)$ was first carried out by Wigner [61]

$$D^{\lambda_\xi}_{m_\xi \widetilde{m}_\xi}(\Omega) = \exp\left(m_\xi \Phi + \widetilde{m}_\xi \Psi\right) \overline{P^{\lambda_\xi}_{m_\xi \widetilde{m}_\xi}(\cos\Theta)}. \tag{2.5}$$

The properties of $P^{\lambda_\xi}_{m_\xi \widetilde{m}_\xi}(z)$ were comprehensively studied by Vilenkin [62, p. 121]. Particularly, for arbitrary $k \in \mathbb{Z}^+$ or $k \in \mathbb{Q}^+ = \{r + 1/2, r \in \mathbb{Z}^+\}$ and $q, q' = -k, -k+1, \ldots, k-1, k$, $P^k_{qq'}(z)$ can be represented by

$$\begin{aligned} P^k_{qq'}(z) =& (-1)^{q-q'} a(k,q,q') \left(\frac{1-z}{1+z}\right)^{\frac{q-q'}{2}} \left(\frac{1+z}{2}\right)^k \\ &\times \sum_{p=\max(0, q-q')}^{\min(k-q', k+q)} b_p(k,q,q') \left(\frac{1-z}{1+z}\right)^p, \end{aligned} \tag{2.6}$$

$$a(k,q,q') \stackrel{\text{def}}{=} \mathrm{i}^{q'-q} \sqrt{(k+q)!(k-q)!(k+q')!(k-q')!}, \tag{2.7}$$

$$b_p(k,q,q') \stackrel{\text{def}}{=} \frac{(-1)^p}{p!(p+q'-q)!(k+q-p)!(k-q'-p)!}. \tag{2.8}$$

Eq. (2.4) associated to any finite unitary group G has a significant meaning in representation theory as well as in theoretical atomic spectroscopy. First of all, it allows one to find a convenient basis for which the matrix elements in Eq. (2.3) appropriate the simplest form [63].

Secondly, for a particular $G = \mathrm{SU}(2)$, the Kronecker product of irreducible matrix representations is reduced in accordance with the rule $D^{\lambda_\xi}(g) \times D^{\lambda_\zeta}(g) = \oplus_\lambda D^{\lambda}(g)$ which makes it possible to form the basis of the type

$$\Phi(\lambda_\xi \lambda_\zeta \lambda m | \widehat{x}_\xi, \widehat{x}_\zeta) = \sum_{m_\xi m_\zeta} \phi(\lambda_\xi m_\xi | \widehat{x}_\xi) \phi(\lambda_\zeta m_\zeta | \widehat{x}_\zeta) \langle \lambda_\xi m_\xi \lambda_\zeta m_\zeta | \lambda m \rangle \tag{2.9}$$

The coefficient $\langle \lambda_\xi m_\xi \lambda_\zeta m_\zeta | \lambda m \rangle$ that transforms one basis into another is called the Clebsch–Gordan coefficient (CGC) of $\mathrm{SU}(2)$, also denoted as $\left[\begin{smallmatrix} \lambda_\xi & \lambda_\zeta & \lambda \\ m_\xi & m_\zeta & m \end{smallmatrix} \right]$ [10, 12, 64]. The basis constructed by using Eq. (2.9) is convenient to calculate matrix elements if applying the Wigner–Eckart theorem. In order to do so, the Hamiltonian H on $\mathcal{H}$ is represented by the sum of irreducible tensor operators H^Λ that act on the subspaces $\mathcal{H}^\Lambda$ of $\mathcal{H}$. For example, the Hamiltonian H_0 is obtained from H if H is confined to operate on $\mathcal{H}^\Lambda = \mathcal{H}^0$ which is a scalar space spanned by the functions Φ_i. On the other hand, Bhatia et. al. [65, Eq. (47)] demonstrated that the angular part $\Phi(\lambda m | \widehat{x}_1, \widehat{x}_2)$ of two-electron wave function was found to be represented in terms of $D^\lambda_{m\widetilde{m}}(\Omega)$. Conversely, such basis is inconvenient for the application of Wigner–Eckart theorem. Moreover, to calculate matrix elements of irreducible tensor operator H^Λ, the integral of type

$$\iint_{S^2} \mathrm{d}\widehat{x}_1 \mathrm{d}\widehat{x}_2 \overline{D^\lambda_{m\widetilde{m}}(\Omega)} H^\Lambda D^{\lambda'}_{m'\widetilde{m}'}(\Omega) \tag{2.10}$$

must be calculated. The integration becomes complicated since Ω depends on $\widehat{x}_1$, $\widehat{x}_2$. To perform the latter integration, the function $\Omega(\widehat{x}_1, \widehat{x}_2)$ should be found. Afterwards it has to be substituted in Eq. (2.5).

The last simple example suggests that the parametrisation of the irreducible matrix representation $D^\lambda(g)$ by the spherical coordinates of $S^2 \times S^2$ makes sense. Here and elsewhere S^2 denotes a 2–dimensional sphere.

2.2 Coordinate transformations

2.2.1 Spherical functions

Suppose given a map $\Omega\colon\ S^2 \times S^2 \longrightarrow \mathrm{SO}(3)$ represented on $\mathbf{R}^3$, a 3–dimensional vector space, by $\widehat{r}_2 = D(3,2)\widehat{r}_1$, where $\widehat{r}_i = \boldsymbol{r}_i / r_i = (\sin\theta_i \cos\varphi_i \ \ \sin\theta_i \sin\varphi_i \ \ \cos\theta_i)^{\mathrm{T}}$. The 3×3 rotation matrix, $D(3,2) \in \mathrm{SO}(3)$, is parametrised by the Euler angles Φ, Θ, Ψ [63, p. 84, Eqs. (7.24)-(7.25)]. In Ref. [66], it was proved that the map Ω is realised on $S^2 \subset \mathbf{R}^3$ if

$$\Phi = \varphi_2 + \alpha\frac{\pi}{2}, \quad \Theta = \beta(\theta_1 - \gamma\theta_2) + 2\pi n, \quad \Psi = -\varphi_1 + \delta\frac{\pi}{2} + 2\pi n' \tag{2.11}$$

Tab. 1: The values for parameters characteristic to the $\mathrm{SU}(2)$–irreducible matrix representation parametrised by the coordinates of $S^2 \times S^2$

The maps			α	β	γ	δ	n	The maps		α	β	γ	δ	n
$\Omega_1^\pm$	Ω_1^+	Ω_{11}^+	+	+	+	−	0	$\Omega_2^\pm$	Ω_2^+	+	+	−	+	0
		Ω_{12}^+	−	+	+	+								
	Ω_1^-	Ω_{11}^-	+	−	+	−			Ω_2^-	−	−	−	−	1
		Ω_{12}^-	−	−	+	+								

with $n, n' \in \mathbb{Z}^+$. The parameters α, β, γ, δ, n are presented in Tab. 1. Then the spherical function $D^k_{qq'}(\Omega)$ is parametrised as follows

$$\begin{aligned}(n, n'; \alpha, \beta, \gamma, \delta | \widehat{x}_1, \widehat{x}_2)^k_{qq'} =& \mathrm{i}^{\alpha q + \delta q'} (-1)^{2(nk + n'q')} \beta^{q'-q} a(k,q,q') \mathrm{e}^{\mathrm{i}(q\varphi_2 - q'\varphi_1)} \{\cos[\tfrac{1}{2}(\theta_1 - \gamma\theta_2)]\}^{2k} \\ & \times \sum_p b_p(k,q,q') \{\tan[\tfrac{1}{2}(\theta_1 - \gamma\theta_2)]\}^{2p+q'-q}.\end{aligned} \tag{2.12}$$

2.2.1 Remark. The exploitation of Euler's formula for the parameter $(\theta_1 - \gamma\theta_2)/2$ indicates the following alternative of parametrisation

$$\begin{aligned}(n,n';\alpha,\beta,\gamma,\delta|\widehat{x}_1,\widehat{x}_2)^k_{qq'} =& \frac{1}{4^k}\mathrm{i}^{(\alpha-1)q+(\delta+1)q'}(-1)^{2(nk+n'q')}\beta^{q'-q}a(k,q,q')h(q,q') \\ &\times\sum_{rs}(-1)^r W^k_{rs}(q-q')\exp\{\mathrm{i}[(r+s-k)\theta_1 - q'\varphi_1]\} \\ &\times\exp\{-\mathrm{i}[(r+s-k)\gamma\theta_2 - q\varphi_2]\},\end{aligned} \tag{2.13}$$

$$\begin{aligned}W^k_{rs}(q-q') \overset{\text{def}}{=} [1+\pi(q,q')]&\binom{q-q'}{s}\binom{2k-q+q'}{r}\frac{\theta(q-q')}{(k-q)!(k+q')!(q-q')!} \\ &\times\ {}_6F_5\left[\begin{matrix}-k+q & -k-q' & \frac{1}{2}(q-q'+1) & \frac{1}{2}(q-q'+2) \\ q-q' & \frac{1}{2}(q-q'-2k) & \frac{1}{2}(q-q'-2k+1) & \\ \frac{1}{2}(q-q'+r-2k) & \frac{1}{2}(q-q'+r-2k+1) & & \\ \frac{1}{2}(q-q'-s+1) & \frac{1}{2}(q-q'-s+2) & & \end{matrix};1\right].\end{aligned} \tag{2.14}$$

The function $h(q,q') = 1$ if $q \neq q'$, otherwise $h(q,q) = 1/2$. The quantity $\theta(q-q')$ denotes the Heaviside step function. The permutation operator $\pi(q,q')$ reverses q and q' that are on the right hand side of $\pi(q,q')$.

Proof. The Euler's formula for $x \in \mathbb{R}$ reads $\mathrm{e}^{\mathrm{i}x} = \cos x + \mathrm{i}\sin x$. Deduce

$$\sin^\alpha x = \left(\frac{\mathrm{i}}{2}\right)^\alpha\sum_{s=0}^{\alpha}(-1)^s\binom{\alpha}{s}\mathrm{e}^{\mathrm{i}(2s-\alpha)x}, \quad \cos^\beta x = \left(\frac{1}{2}\right)^\beta\sum_{r=0}^{\beta}\binom{\beta}{r}\mathrm{e}^{\mathrm{i}(2r-\beta)x},$$

where the binomial formula for $(\mathrm{e}^{\mathrm{i}x} \pm \mathrm{e}^{-\mathrm{i}x})^y$ has been used. In this case (see Eq. (2.12)),

$$x = \tfrac{1}{2}(\theta_1 - \gamma\theta_2), \quad \alpha = 2p + q' - q, \quad \beta = 2k - 2p - q' + q.$$

These values are substituted in Eq. (2.12). The exponents with the parameters p vanish since $\alpha \propto +2p$ and $\beta \propto -2p$. In addition, the summation over p can be proceeded for the construction

$$\sum_p(-1)^p b_p(k,q,q')\binom{2p+q'-q}{s}\binom{2k-2p-q'+q}{r}.$$

By passing to Eq. (2.8), we get for $q \geq q'$, the binomial series

$$\begin{aligned}&\binom{q-q'}{s}\binom{2k-q+q'}{r}\frac{1}{(k-q)!(k+q')!(q-q')!} \\ &\times\ {}_6F_5\left[\begin{matrix}-k+q & -k-q' & \frac{1}{2}(q-q'+1) & \frac{1}{2}(q-q'+2) \\ q-q' & \frac{1}{2}(q-q'-2k) & \frac{1}{2}(q-q'-2k+1) & \\ \frac{1}{2}(q-q'+r-2k) & \frac{1}{2}(q-q'+r-2k+1) & & \\ \frac{1}{2}(q-q'-s+1) & \frac{1}{2}(q-q'-s+2) & & \end{matrix};1\right].\end{aligned}$$

If $q \leq q'$, the last expression remains irrelevant if replacing q with q'. Thus for any q, q', it is convenient to use the Heaviside step functions $\theta(q-q')$ and $\theta(q'-q)$. This proves Remark 2.2.1. □

If follows from Eqs. (2.12)-(2.13) and Tab. 1 that the four spherical functions on $S^2 \times S^2$ serve for the irreducible matrix representation $D^k_{qq'}(\Omega)$. Each of the function corresponds to $D^k_{qq'}(\Omega)$ in distinct areas of S^2. The spherical functions are considered as follows

$${}^+\xi^k_{qq'}(\widehat{x}_1,\widehat{x}_2): \begin{cases}\mathcal{L}^2(\Omega^+_{11}) \overset{\text{def}}{=} \{\varphi_2 \in [0,\pi];\theta_2 \in [0,\theta_1], n' = 1,2\} \\ \mathcal{L}^2(\Omega^-_{12}) \overset{\text{def}}{=} \{\varphi_2 \in [\pi,2\pi];\theta_2 \in [\theta_1,\pi], n' = 0,1\}\end{cases}, \tag{2.15a}$$

$$ {}^{-}\xi^{k}_{qq'}(\widehat{x}_1,\widehat{x}_2):\quad \begin{cases} \mathcal{L}^2(\Omega^{-}_{11}) \stackrel{\text{def}}{=} \{\varphi_2\in[0,\pi];\theta_2\in[\theta_1,\pi],n'=1,2\} \\ \mathcal{L}^2(\Omega^{+}_{12}) \stackrel{\text{def}}{=} \{\varphi_2\in[\pi,2\pi];\theta_2\in[0,\theta_1],n'=0,1\} \end{cases}, \tag{2.15b} $$

$$ {}^{+}\zeta^{k}_{qq'}(\widehat{x}_1,\widehat{x}_2):\quad \mathcal{L}^2(\Omega^{+}_{2}) \stackrel{\text{def}}{=} \{\varphi_2\in[0,3\pi/2];\theta_2\in\mathcal{M}^{+}_{\theta_1},n'=0,1\}, \tag{2.15c} $$

$$ {}^{-}\zeta^{k}_{qq'}(\widehat{x}_1,\widehat{x}_2):\quad \mathcal{L}^2(\Omega^{-}_{2}) \stackrel{\text{def}}{=} \{\varphi_2\in[\pi/2,2\pi];\theta_2\in\mathcal{M}^{-}_{\theta_1},n'=1,2\}. \tag{2.15d} $$

The compacts $\mathcal{M}^{\pm}_{\theta_1}\subseteq[0,\pi]$ are defined by

$$ \mathcal{M}^{+}_{\theta_1}\stackrel{\text{def}}{=}\begin{cases}(0,\pi], & \theta_1=0,\\ 0, & \theta_1=\pi,\\ (0,\pi-\theta_1], & \theta_1\in(0,\pi),\end{cases} \qquad \mathcal{M}^{-}_{\theta_1}\stackrel{\text{def}}{=}\begin{cases}\pi, & \theta_1=0,\\ [0,\pi], & \theta_1=\pi,\\ [\pi-\theta_1,\pi], & \theta_1\in(0,\pi).\end{cases} \tag{2.16} $$

The spherical functions are related to each other by the phase factors: ${}^{-}\xi^{k}_{qq'}=(-1)^{q-q'}\,{}^{+}\xi_{qq'}$, ${}^{-}\zeta^{k}_{qq'}=(-1)^{2q'}\,{}^{+}\zeta^{k}_{qq'}$. If

$$ {}^{\pm}\tau^{k}_{qq'}\in\{\eta^{k}_{qq'},\ {}^{\pm}\zeta^{k}_{qq'}\},\quad \eta^{k}_{qq'}\in\{{}^{+}\xi^{k}_{qq'},\ {}^{-}\xi^{k}_{qq'}\}, \tag{2.17} $$

then the functions ${}^{\pm}\tau^{k}_{qq'}$ satisfy

$$ \sum_{q}{}^{+}\tau^{k}_{qq'}\,{}^{-}\tau^{k}_{-q-q''}=\delta_{q'q''},\quad \overline{{}^{\pm}\tau^{k}_{qq'}}=(-1)^{q-q'}\,{}^{\pm}\tau^{k}_{-q-q'}. \tag{2.18} $$

The products of spherical functions are reducible by using the rule ${}^{\pm}\tau^{k_1}\times{}^{\pm}\tau^{k_2}=\oplus_k\,{}^{\pm}\tau^{k}$, which is obvious since the ${}^{\pm}\tau^{k}(\widehat{x}_1,\widehat{x}_2)$ represent the $D^k(\Omega)$ in different areas $\mathcal{L}^2(\Omega)\subset S^2$.

Example. Assume that $\widehat{x}_1=(\pi/6,\pi/4)$ and $\widehat{x}_2=(\pi/3,\pi)$. Possible rotations are realised on S^2 by the angles $\Omega^{-}_{11}=(3\pi/2,\pi/6,5\pi/4)$ and $\Omega^{+}_{2}=(3\pi/2,\pi/2,\pi/4)$. In accordance with Eq. (2.15), for $k=5/2$, $q=-1/2$, $q'=3/2$, the functions are

$$ {}^{-}\xi^{5/2}_{-1/2\,3/2}(\pi/6,\pi/4,\pi/3,\pi)=D^{5/2}_{-1/2\,3/2}(3\pi/2,\pi/6,5\pi/4)=1/32\,(-1)^{1/8}(13-3\sqrt{3}), $$
$$ {}^{+}\zeta^{5/2}_{-1/2\,3/2}(\pi/6,\pi/4,\pi/3,\pi)=D^{5/2}_{-1/2\,3/2}(3\pi/2,\pi/2,\pi/4)=(-1)^{5/8}\,1/4. $$

Obtained spherical functions ${}^{\pm}\tau^{k}_{qq'}(\widehat{x}_1,\widehat{x}_2)$ are suitable for their direct realisation through Eq. (2.4) which also makes it possible to carry out the integration in Eq. (2.10) easily enough.

2.2.2 RCGC technique

It is natural to make use of the spherical functions ${}^{\pm}\tau^{\lambda}_{\mu\nu}(\widehat{x}_1,\widehat{x}_2)$ in selection of a convenient basis, as described in Eq. (2.4). The argument becomes more motivated recalling that the irreducible tensor operators T^{λ}—being of special interest in atomic physics—also transform under the irreducible matrix representations $D^{\lambda}(\Omega)$. In general, the $2\lambda+1$ components T^{λ}_{μ} of T^{λ} on $\mathcal{H}^{\lambda}$ transform under the unitary matrix representation $D^{\lambda}(g)$ as follows [64, p. 70, Eq. (3.57)]

$$ T^{\lambda\dagger}_{\nu}T^{\lambda}_{\mu}T^{\lambda}_{\nu}=\sum_{\rho}D^{\lambda}_{\mu\rho}(g)T^{\lambda}_{\rho}. \tag{2.19} $$

It is assumed that each invariant subspace $\mathcal{H}^{\lambda}$ is spanned by the orthonormal basis $\phi(\lambda\mu|\widehat{x}_{\mu})$, for which Eq. (2.4) holds true. Alike the case of the basis in Eq. (2.9), for $G=\mathrm{SU}(2)$, Eq. (2.19) allows each tensor product $T^{\lambda_1}\times T^{\lambda_2}$ to be reduced by

$$ [T^{\lambda_1}\times T^{\lambda_2}]^{\lambda}_{\mu}=\sum_{\mu_1\mu_2}T^{\lambda_1}_{\mu_1}T^{\lambda_2}_{\mu_2}\langle\lambda_1\mu_1\lambda_2\mu_2|\lambda\mu\rangle, \tag{2.20} $$

where the irreducible tensor operator $[T^{\lambda_1}\times T^{\lambda_2}]^{\lambda}$ transforms under $D^{\lambda}(\Omega)$.

Most of the physical operators T^{λ}—basically studied in atomic spectroscopy—are expressed in terms of D^{λ} and their various combinations. These are, for example, the normalised spherical

harmonics $C^k_q(\widehat{x}) = \mathrm{i}^k D^k_{q0}(\bar{\Omega})$, $\bar{\Omega} = (\Phi, \Theta, 0)$ with $\Phi = \varphi + \pi/2$, $\Theta = \theta$; the spherical harmonics $Y^k_q(\widehat{x}) = \sqrt{(2k+1)/4\pi} C^k_q(\widehat{x})$. The spin operator S^1, the angular momentum operator L^1 are also expressed in terms of the irreducible matrix representation D^1, as it was demonstrated in Refs. [52, 67]. The announced particular cases of T^λ represent the operators that depend on the coordinate system. Being more tight, these spherical tensor operators are in turn the functions of $\widehat{x} \equiv \theta\varphi$. With this in mind, we may write

$$T^\lambda_\mu(\widehat{x}_2) = \sum_\rho {}^{\pm}\tau^\lambda_{\mu\rho}(\widehat{x}_1, \widehat{x}_2) T^\lambda_\rho(\widehat{x}_1). \tag{2.21}$$

Eq. (2.21) also applies for the basis $\phi(\lambda\mu|\widehat{x}_2)$. Then the following result is immediate

$$\Phi(\lambda_1\lambda_2\lambda\mu|\widehat{x}_1, \widehat{x}_2) = \sum_{\widetilde{\lambda}\nu} \begin{pmatrix} \widetilde{\lambda} & \lambda_1\lambda_2\lambda \\ \nu & \mu \end{pmatrix}; \widehat{x}_1, \widehat{x}_2 \Bigg) \bar{\Phi}(\lambda_1\lambda_2\widetilde{\lambda}\nu|\widehat{x}_1), \tag{2.22}$$

$$\begin{pmatrix} \widetilde{\lambda} & \lambda_1\lambda_2\lambda \\ \nu & \mu \end{pmatrix}; \widehat{x}_1, \widehat{x}_2 \Bigg) \stackrel{\text{def}}{=} \sum_{\mu_1\mu_2} \begin{pmatrix} \lambda_1 & \lambda_2 & \widetilde{\lambda} \\ \mu_1 & \mu_2 & \nu \end{pmatrix}; \widehat{x}_1, \widehat{x}_2 \Bigg) \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda \\ \mu_1 & \mu_2 & \mu \end{bmatrix}, \tag{2.23}$$

$$\begin{pmatrix} \lambda_1 & \lambda_2 & \widetilde{\lambda} \\ \mu_1 & \mu_2 & \nu \end{pmatrix}; \widehat{x}_1, \widehat{x}_2 \Bigg) \stackrel{\text{def}}{=} \sum_{\widetilde{\mu}_2} {}^{\pm}\tau^{\lambda_2}_{\mu_2\widetilde{\mu}_2}(\widehat{x}_1, \widehat{x}_2) \begin{bmatrix} \lambda_1 & \lambda_2 & \widetilde{\lambda} \\ \mu_1 & \widetilde{\mu}_2 & \nu \end{bmatrix}, \tag{2.24}$$

where the basis $\Phi(\lambda_1\lambda_2\lambda\mu|\widehat{x}_1, \widehat{x}_2)$ is defined in Eq. (2.9) and $\bar{\Phi}(\lambda_1\lambda_2\widetilde{\lambda}\nu|\widehat{x}_1) \equiv \Phi(\lambda_1\lambda_2\widetilde{\lambda}\nu|\widehat{x}_1, \widehat{x}_1)$ is the transformed basis. The quantities $\left(\begin{smallmatrix} \lambda_1 & \lambda_2 & \widetilde{\lambda} \\ \mu_1 & \mu_2 & \nu \end{smallmatrix}; \widehat{x}_1, \widehat{x}_2\right)$ and $\left(\begin{smallmatrix} \widetilde{\lambda} & \lambda_1\lambda_2\lambda \\ \nu & \mu \end{smallmatrix}; \widehat{x}_1, \widehat{x}_2\right)$ are called rotated Clebsch–Gordan coefficients (RCGC) of the first and second type [66, Sec. 6], respectively. Particularly,

$$\begin{pmatrix} \lambda_1 & \lambda_2 & \widetilde{\lambda} \\ \mu_1 & \mu_2 & \nu \end{pmatrix}; \widehat{x}_1, \widehat{x}_1 \Bigg) = \begin{bmatrix} \lambda_1 & \lambda_2 & \widetilde{\lambda} \\ \mu_1 & \mu_2 & \nu \end{bmatrix}, \quad \begin{pmatrix} \widetilde{\lambda} & \lambda_1\lambda_2\lambda \\ \nu & \mu \end{pmatrix}; \widehat{x}_1, \widehat{x}_1 \Bigg) = \delta_{\lambda\widetilde{\lambda}}\delta_{\mu\nu}. \tag{2.25}$$

The RCGCs are reducible. For example,

$$\begin{pmatrix} \lambda_1 & \lambda_2 & \lambda \\ \mu_1 & \mu_2 & \mu \end{pmatrix}; \widehat{x}_1, \widehat{x}_2 \Bigg) \begin{pmatrix} \widetilde{\lambda}_1 & \widetilde{\lambda}_2 & \widetilde{\lambda} \\ \nu_1 & \nu_2 & \nu \end{pmatrix}; \widehat{x}_1, \widehat{x}_2 \Bigg) = \frac{(-1)^{\widetilde{\lambda}_2+1}}{[\widetilde{\lambda}_2]^{1/2}} \sum_{\Lambda_2} (-1)^{\Lambda_2} [\Lambda_2]^{1/2} \sum_{\rho_2\widetilde{\rho}_2} (-1)^{\widetilde{\rho}_2}$$
$$\times \begin{pmatrix} \lambda_2 & \Lambda_2 & \widetilde{\lambda}_2 \\ -\rho_2 & M_2 & \widetilde{\rho}_2 \end{pmatrix}; \widehat{x}_1, \widehat{x}_2 \Bigg) \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda \\ \mu_1 & \rho_2 & \mu \end{bmatrix} \begin{bmatrix} \widetilde{\lambda}_1 & \widetilde{\lambda}_2 & \widetilde{\lambda} \\ \nu_1 & \widetilde{\rho}_2 & \nu \end{bmatrix} \begin{bmatrix} \lambda_2 & \widetilde{\lambda}_2 & \Lambda_2 \\ \mu_2 & \nu_2 & M_2 \end{bmatrix}. \tag{2.26}$$

The abbreviation $[x]^{1/2} \equiv \sqrt{2x+1}$.

> The specific feature of technique based on the coordinate transformations (or simply RCGC technique) is the ability to transform the coordinate-dependence of the basis $\Phi(\Gamma\Pi\Lambda M|\widehat{x}_1, \widehat{x}_2, \ldots, \widehat{x}_N)$ in $\mathcal{H}^\Lambda$ preserving its inner structure. The transformed basis $\bar{\Phi}(\widetilde{\Gamma}\widetilde{\Pi}\widetilde{\Lambda}\widetilde{M}|\widehat{x}_\xi)$ in $\mathcal{H}^{\widetilde{\Lambda}}$ implicates the tensor structure of the initial basis $\Phi(\Gamma\Pi\Lambda M|\widehat{x}_1, \widehat{x}_2, \ldots, \widehat{x}_N)$, but the coordinate-dependence is represented by the function of arbitrary variable $\widehat{x}_\xi$, where ξ acquires any value from $1, 2, \ldots, N$.

A particular case of the two-electron basis function in Eq. (2.22) along with the properties of RCGCs (see Eqs. (2.25)-(2.26)) initiates a possibility to change the calculation of multiple integrals with the calculation of a single one. This argument also fits the integrals of the type in Eq. (2.10). In a two-electron case, a simple evaluation indicates that the integration of the operator $[T^{k_1}(\widehat{x}_1) \times T^{k_2}(\widehat{x}_2)]^k$ (see Eq. (2.20)) on the basis $\Phi(\lambda_1\lambda_2\lambda\mu|\widehat{x}_1, \widehat{x}_2)$ (see Eq. (2.9)) is transformed into a single integral of the transformed operator $[T^{\widetilde{k}_1}(\widehat{x}_1) \times T^{\widetilde{k}_2}(\widehat{x}_1)]^{\widetilde{k}}$ on the transformed basis $\bar{\Phi}(\widetilde{\lambda}_1\widetilde{\lambda}_2\widetilde{\lambda}\widetilde{\mu}|\widehat{x}_1)$. The obtained single integral becomes even simpler if T^k acquires some special values. For instance, if $T^k \equiv C^k$, then the transformed operator equals to $\mathrm{i}^{\widetilde{k}_1+\widetilde{k}_2-\widetilde{k}} C^{\widetilde{k}}(\widehat{x}_1)\langle\widetilde{k}_1 0\widetilde{k}_2 0|\widetilde{k}0\rangle$. Moreover, if the basis $\phi(\lambda_1\mu_1|\widehat{x}_1)$ is written in terms of $D^{\lambda_1}_{\mu_1 0}(\bar{\Omega}_1)$ [67, Eq. (38)], then the transformed basis reads $D^{\widetilde{\lambda}}_{\widetilde{\mu}0}(\bar{\Omega}_1)\langle\widetilde{\lambda}_1 0\widetilde{\lambda}_2 0|\widetilde{\lambda}0\rangle$. In addition, due to transformations, the three RCGCs II arise (see Eqs. (2.22)-(2.23)). Their product is

reduced in accordance with Eqs. (2.23), (2.26). The obtained RCGC II $\left(\begin{smallmatrix}\widetilde{\Lambda} & \Lambda_1\Lambda_2\Lambda \\ \widetilde{\epsilon} & \epsilon\end{smallmatrix}; \widehat{x}_1, \widehat{x}_2\right)$ is integrated over $\widehat{x}_2$, and the resultant function also depends on $\widehat{x}_1$ only. It goes without saying that the procedure of integration is suitable for the N–electron case. However, to improve the applicability of this algorithm, the integrals of the RCGCs or, what is equivalent, the integrals of spherical functions ${}^{\pm}\tau^k_{qq'}(\widehat{x}_1, \widehat{x}_2)$ should be calculated.

In Ref. [66, Sec. 5], it was proved that the integral of ${}^{\pm}\tau^k_{qq'}(\widehat{x}_1, \widehat{x}_2)$ over $\widehat{x}_2 \in S^2$ is the sum of integrals determined in the areas $\mathcal{L}^2(\Omega)$. That is,

$$\begin{aligned}\mathcal{S}^k_{qq'}(\widehat{x}_1) = &\left(\int_{\mathcal{L}^2(\Omega^+_{11})} + \int_{\mathcal{L}^2(\Omega^-_{12})}\right) \mathrm{d}\widehat{x}_2 \; {}^{+}\xi^k_{qq'}(\widehat{x}_1, \widehat{x}_2) \\ &+ \left(\int_{\mathcal{L}^2(\Omega^-_{11})} + \int_{\mathcal{L}^2(\Omega^+_{12})}\right) \mathrm{d}\widehat{x}_2 \; {}^{-}\xi^k_{qq'}(\widehat{x}_1, \widehat{x}_2), \end{aligned} \tag{2.27}$$

where the measure $\mathrm{d}\widehat{x}_2 = \mathrm{d}\varphi_2 \mathrm{d}\theta_2 \sin\theta_2$; a normalisation $\int_{S^2} \mathrm{d}\widehat{x}_2 = 4\pi$. A direct integration leads to

$$\begin{aligned}\mathcal{S}^k_{qq'}(\widehat{x}_1) =& \lambda_{q'}(\varphi_1) \mathrm{i}^{q-q'-1} \frac{(-1)^q - 1}{q} \big((-1)^{q'} + 1\big) a(k, q, q') \mathrm{e}^{-\mathrm{i}q'\varphi_1} \\ &\times \sum_p b_p(k, q, q') \big({}_pI^k_{qq'}(\theta_1; 0, \theta_1) + (-1)^{q-q'} \, {}_pI^k_{qq'}(\theta_1; \theta_1, \pi)\big). \end{aligned} \tag{2.28}$$

The functions $\lambda_{q'}(\varphi_1)$ and ${}_pI^k_{qq'}(\theta_1; a, b)$ are defined by

$$\lambda_{q'}(\varphi_1) \stackrel{\text{def}}{=} \begin{cases} (-1)^{q'}, & \varphi_1 \in [0, \pi/2] \\ (-1)^{2q'}, & \varphi_1 \in (\pi/2, 3\pi/2] \\ (-1)^{3q'}, & \varphi_1 \in (3\pi/2, 2\pi] \end{cases}, \tag{2.29}$$

$${}_pI^k_{qq'}(\theta_1; a, b) \stackrel{\text{def}}{=} 2\big\{2I^p_1(a, b)\cos\theta_1 + (I^p_2(a, b) - I^p_0(a, b))\sin\theta_1\big\}, \tag{2.30}$$

$$I^p_s(a, b) \stackrel{\text{def}}{=} I^p_s(\tan[\tfrac{1}{2}(\theta_1 - b)]) - I^p_s(\tan[\tfrac{1}{2}(\theta_1 - a)]), \quad s = 0, 1, 2, \tag{2.31}$$

$$\begin{aligned} I^p_s(z) \stackrel{\text{def}}{=}& \frac{z^{2p+q'-q+s+1}}{2p + q' - q + s + 1} \\ &\times {}_2F_1\left(\frac{2p + q' - q + s + 1}{2}, k + 2; \frac{2p + q' - q + s + 3}{2}; -z^2\right). \end{aligned} \tag{2.32}$$

It appears from Eqs. (2.28)-(2.32) that the function $\mathcal{S}^k_{qq'}(\widehat{x})$ is represented by the sum of Gauss's hypergeometric functions. If, particularly, $l \in \mathbb{Z}^+$, then $\mathcal{S}^l_{\mu m}(\widehat{x}) = \delta_{\mu 0}\mathcal{S}^l_{0m}(\widehat{x})$. Indeed, it follows from Eq. (2.28) that for $l \in \mathbb{Z}^+$,

$$\mathcal{S}^l_{0m}(\widehat{x}) = 2\pi l! \sqrt{(l+m)!(l-m)!}\mathrm{e}^{-\mathrm{i}m\varphi} \sum_{p=\max(0,-m)}^{\min(l,l-m)} \frac{(-1)^p \, {}_pI^l_{0m}(\theta; 0, \pi)}{p!(p+m)!(l-p)!(l-m-p)!}. \tag{2.33}$$

2.2.2 Definition. The functions

$$\mathcal{S}^l_m(\widehat{x}) \stackrel{\text{def}}{=} \mathcal{S}^l_{0m}(\widehat{x}) \tag{2.34}$$

with $l \in \mathbb{Z}^+$ form the set L_l such that the cardinality $\#L_l \stackrel{\text{def}}{=} 2l + 1$, and the indices satisfy $m = -l, -l+1, \ldots, l-1, l$.

2.2.3 Proposition. *For $l \in \mathbb{Z}^+$, the $\#L_l$ functions $\mathcal{S}^l_m(\widehat{x})$ constitute a set L_l of components of the $\mathrm{SO}(3)$–irreducible tensor operator $\mathcal{S}^l(\widehat{x})$.*

Proof. To prove the proposition, it suffices to demonstrate that $\mathcal{S}^l_m(\widehat{x})$ transforms under $D^l(\Omega)$ (see Eq. (2.19)) or, equivalently, under $\eta^l(\widehat{x}_1, \widehat{x}_2)$ (see Eqs. (2.17)-(2.21)), where the square matrix $\eta^l(\widehat{x}_1, \widehat{x}_2) \in \{{}^{+}\xi^l(\widehat{x}_1, \widehat{x}_2), \; {}^{-}\xi^l(\widehat{x}_1, \widehat{x}_2)\}$.

To begin with, integrate both sides of Eq. (2.21) over $\widehat{x}_2$ on S^2. For positive integer $\lambda \equiv l$, the result reads

$$\int_{S^2} \mathrm{d}\widehat{x}_2\, T^l_\mu(\widehat{x}_2) = \delta_{\mu 0} \sum_{\rho=-l}^{l} \mathcal{S}^l_\rho(\widehat{x}_1) T^l_\rho(\widehat{x}_1), \tag{2.35}$$

The left hand side of Eq. (2.35) does not depend on $\widehat{x}_1$ and it is a function of l. This implies that the relation

$$\sum_{\rho=-l}^{l} \mathcal{S}^l_\rho(\widehat{x}_1) T^l_\rho(\widehat{x}_1) = \sum_{\rho=-l}^{l} \mathcal{S}^l_\rho(\widehat{x}_2) T^l_\rho(\widehat{x}_2)$$

is valid for any $\widehat{x}_1, \widehat{x}_2 \in S^2$. Apply Eq. (2.21) for $T^l_\rho(\widehat{x}_2)$ once again. Then

$$\sum_{\rho=-l}^{l} \mathcal{S}^l_\rho(\widehat{x}_1) T^l_\rho(\widehat{x}_1) = \sum_{\rho,\nu=-l}^{l} \mathcal{S}^l_\rho(\widehat{x}_2) \eta^l_{\rho\nu}(\widehat{x}_1, \widehat{x}_2) T^l_\nu(\widehat{x}_1).$$

Finally, replace ρ with ν on the right hand side and list the common terms next to $T^l_\rho(\widehat{x}_1)$ from both sides of expression. After replacing $\widehat{x}_1$ with $\widehat{x}_2$, the result reads

$$\mathcal{S}^l_\rho(\widehat{x}_2) = \sum_{\nu=-l}^{l} \eta^l_{\nu\rho}(\widehat{x}_2, \widehat{x}_1) \mathcal{S}^l_\nu(\widehat{x}_1), \quad \rho = -l, -l+1, \ldots, l-1, l. \tag{2.36}$$

This proves the proposition. □

According to Proposition 2.2.3, the tensor products of $\mathrm{SO}(3)$–irreducible tensor operators $\mathcal{S}^l(\widehat{x})$ are reduced by using Eq. (2.20).

Conjecture. Unlike the case of $\mathrm{SO}(3)$, the transformation properties of functions $\mathcal{S}^k_{qq'}(\widehat{x})$ with rational numbers $k \in \mathbb{Q}^+$ are not so clear. In this case, Eq. (2.36) is not valid. This is because a direct integration, as in Eq. (2.35), over $\widehat{x}_2$ on S^2 can not be performed correctly due to the specific properties of $\mathcal{S}^k_{qq'}(\widehat{x})$ for $k \in \mathbb{Q}^+$. That is, for $l \in \mathbb{Z}^+$,

$$\mathcal{S}^l_m(\widehat{x}_1) \stackrel{\text{def}}{=} \int_{S^2} \mathrm{d}\widehat{x}_2\, \eta^l_{0m}(\widehat{x}_1, \widehat{x}_2)$$

for any $\widehat{x}_1 \in S^2$. To compare with, see Eq. (2.27). This means, Eq. (2.21) applies for $\eta^l_{\mu\rho}(\widehat{x}_1, \widehat{x}_2) \in \{ {}^{+}\xi^l_{\mu\rho}(\widehat{x}_1, \widehat{x}_2),\ {}^{-}\xi^l_{\mu\rho}(\widehat{x}_1, \widehat{x}_2)\}$, for all integers μ, ρ and for all possible $\widehat{x}_1$, $\widehat{x}_2$. Conversely, for $k \in \mathbb{Q}^+$, the latter expression does not fit, as q, q' are the rational numbers. However, the numerical analysis enforces to make a prediction that particularly

$$S^k_{qq'}(\widehat{x}_2; \xi) = -\sum_{Q=-k}^{k} {}^{+}\xi^k_{Qq'}(\widehat{x}_2, \widehat{x}_1) S^k_{qQ}(\widehat{x}_1; \xi), \quad \mathcal{S}^k_{qq'}(\widehat{x}_1; \xi) \stackrel{\text{def}}{=} \int_{S^2} \mathrm{d}\widehat{x}_2\, {}^{+}\xi^k_{qq'}(\widehat{x}_1, \widehat{x}_2).$$

Knowing the connection between $\mathrm{SO}(3)$ and $\mathrm{SU}(2)$, it turns out that there must exist the transformation properties for $S^k_{qq'}$ with $k \in \mathbb{Q}^+$, similar to Eq. (2.36) and to this day, the $\mathrm{SU}(2)$ case is an open question yet.

Having defined the functions $\mathcal{S}^k_{qq'}(\widehat{x})$, the calculation of integrals in Eq. (2.10) requires little effort. Besides, this is a simpler case than the integration on the basis $\Phi(\Gamma\Pi\Lambda M|\widehat{x}_1, \widehat{x}_2, \ldots, \widehat{x}_N)$ since the product of $\overline{D^\lambda_{m\widetilde{m}}(\Omega)}$ and $D^{\lambda'}_{m'\widetilde{m}'}(\Omega)$ is reduced to a single spherical function $D^\Lambda_{M\widetilde{M}}(\Omega)$ which is replaced by ${}^{\pm}\tau^\Lambda_{M\widetilde{M}}(\widehat{x}_1, \widehat{x}_2)$. If H^Λ represents the angular part $(C^k(\widehat{x}_1) \cdot C^k(\widehat{x}_2))$ of the Coulomb interaction operator $1/r_{12}$, then $\Lambda = 0$ and a double integral is transformed to a single one as follows

$$\iint_{S^2} \mathrm{d}\widehat{x}_1\,\mathrm{d}\widehat{x}_2\;\overline{D^l_{m\widetilde{m}}(\Omega)}(C^k(\widehat{x}_1)\cdot C^k(\widehat{x}_2))D^{l'}_{m'\widetilde{m}'}(\Omega) = 4\pi[k]^{-1/2}(-1)^{k+m'+\widetilde{m}}$$
$$\times\sum_K [K]^{-1/2}[k\|\mathcal{S}^K\|k]\sum_L \begin{bmatrix} l & l' & L \\ -m & m' & m'-m\end{bmatrix}\begin{bmatrix} l & l' & L \\ -\widetilde{m} & \widetilde{m}' & \widetilde{m}'-\widetilde{m}\end{bmatrix}\begin{bmatrix} L & k & K \\ m'-m & m-m' & 0\end{bmatrix}$$
$$\times\sum_{Q=\text{even}}\begin{bmatrix} k & k & K \\ m'-m & Q+m-m' & Q\end{bmatrix}\begin{bmatrix} L & k & K \\ \widetilde{m}'-\widetilde{m} & \widetilde{m}-\widetilde{m}'-Q & -Q\end{bmatrix}. \qquad (2.37)$$

Tab. 2: Numerical values of reduced matrix element of SO(3)–irreducible tensor operator $\mathcal{S}^k$ for several integers l, l'

l	l'	k	$(4\pi)^{-1}[l\|\mathcal{S}^k\|l']$	l	l'	k	$(4\pi)^{-1}[l\|\mathcal{S}^k\|l']$	l	l'	k	$(4\pi)^{-1}[l\|\mathcal{S}^k\|l']$
0	0	0	1	2	4	2	$\sqrt{\frac{2}{5\cdot 7}}$	1	5	4	$-\frac{1}{27\sqrt{5}}$
1	1	0	3	1	3	4	$-\frac{2}{5\cdot 27}$	2	4	4	$-\frac{2}{27}\sqrt{\frac{5}{7\cdot 11}}$
1	1	2	$\frac{1}{5}\sqrt{\frac{2}{5}}$	2	2	2	$\frac{1}{3}\sqrt{\frac{2}{7}}$	3	5	2	$\frac{1}{3}\sqrt{\frac{2\cdot 7}{3\cdot 5}}$
1	3	2	$\frac{1}{5}\sqrt{\frac{3}{5}}$	3	3	0	7	4	6	2	$\frac{3}{\sqrt{5\cdot 11}}$

Reduced matrix elements $[l\|\mathcal{S}^k\|l']$ are found from the Wigner–Eckart theorem. That is,

$$[l\|\mathcal{S}^k\|l'] = \frac{[l]^{1/2}}{[l']^{1/2}}[l'\|\mathcal{S}^k\|l] = \sum_{qmm'}\langle lm|\mathcal{S}^k_q|l'm'\rangle\langle l'm'kq|lm\rangle, \qquad (2.38)$$

where the matrix element is calculated on the basis of spherical harmonics. Some of the values of $[l\|\mathcal{S}^k\|l']$ are listed in Tab. 2.

In general, each N-integral

$$\int_{S^2}\mathrm{d}\widehat{x}_1\int_{S^2}\mathrm{d}\widehat{x}_2\ldots\int_{S^2}\mathrm{d}\widehat{x}_N\;\Phi^\dagger(\Gamma^{bra}\Pi^{bra}\Lambda^{bra}M^{bra}|\widehat{x}_1,\widehat{x}_2,\ldots,\widehat{x}_N)T^K_Q(\widehat{x}_1,\widehat{x}_2,\ldots,\widehat{x}_N)$$
$$\times\Phi(\Gamma^{ket}\Pi^{ket}\Lambda^{ket}M^{ket}|\widehat{x}_1,\widehat{x}_2,\ldots,\widehat{x}_N)$$

is replaced by the sum of single integrals

$$\int_{S^2}\mathrm{d}\widehat{x}\;\bar{\Phi}^\dagger(\widetilde{\Gamma}^{bra}\widetilde{\Pi}^{bra}\widetilde{\Lambda}^{bra}\widetilde{M}^{bra}|\widehat{x})\bar{T}^{\widetilde{K}}_{\widetilde{Q}}(\widehat{x})\mathcal{S}^{\Lambda_2}_{M_2M_2'}(\widehat{x})\mathcal{S}^{\Lambda_3}_{M_3M_3'}(\widehat{x})\ldots\mathcal{S}^{\Lambda_N}_{M_NM_N'}(\widehat{x})$$
$$\times\bar{\Phi}(\widetilde{\Gamma}^{ket}\widetilde{\Pi}^{ket}\widetilde{\Lambda}^{ket}\widetilde{M}^{ket}|\widehat{x}).$$

Instead of that the $N-1$ functions $\mathcal{S}$ are produced. At least for $\Lambda_i\in\mathbb{Z}^+\;\forall i=2,3,\ldots,N$, the last integral can acquire the following matrix representation (see Proposition 2.2.3)

$$\langle\widetilde{\Gamma}^{bra}\Pi^{bra}\widetilde{\Lambda}^{bra}\widetilde{M}^{bra}|[\ldots[[\bar{T}^{\widetilde{K}}\times\mathcal{S}^{\Lambda_2}]^{E_2}\times\mathcal{S}^{\Lambda_3}]^{E_3}\times\ldots\times\mathcal{S}^{\Lambda_N}]^{E_N}_{\widetilde{M}_N}|\widetilde{\Gamma}^{ket}\Pi^{ket}\widetilde{\Lambda}^{ket}\widetilde{M}^{ket}\rangle, \qquad (2.39)$$

recalling that the parity is invariant under coordinate transformation. That is, $\Pi^{bra,ket}=\widetilde{\Pi}^{bra,ket}$. Eq. (2.39) represents thus the single-particle matrix element on the basis of transformed functions.

The calculation of spherical tensor operator matrix element on the basis functions $\Phi(\Gamma\Pi\Lambda M|\widehat{x}_1,\widehat{x}_2,\ldots,\widehat{x}_N)$ assigns to calculate the N-integral over the spherical coordinates $\widehat{x}_\xi\;\forall\xi=1,2,\ldots,N$. If the basis is represented in terms of Slater determinants, then a usual technique based on the Wigner–Eckart theorem is convenient. That is, the N–electron matrix element is taken to be the product of single-electron

matrix elements. In the individual cases, the calculation may be performed in a different way. If the RCGC technique is exploited, the N-integral is reduced to the sum of single integrals. The technique based on the coordinate transformations is even more applicable for the basis expressed by the spherical functions $D^{\Lambda}(\Omega)$. The example of helium-like atoms confirms this clearly.

2.3 System of variable particle number

Unlike the case of Slater determinants it is more convenient to form the basis $\Phi(\Gamma\Pi\Lambda M)$ from the single-electron quantum states $|\lambda m\rangle$—known as the vectors of Hilbert space—that are created by the $2\lambda+1$ components of irreducible tensor operator a^{λ}—known as the Fock space operator—acting on the genuine vacuum $|0\rangle$. In this case, the quantum mechanical many-body system is characterised by the number of particles rather than their coordinates. The characteristic operator is the particle number operator $\widehat{N} = -[\lambda]^{1/2} W^{0}(\lambda\widetilde{\lambda})$, where the irreducible tensor operator $W^{\Lambda}(\lambda_1\widetilde{\lambda}_2) = [a^{\lambda_1} \times \tilde{a}^{\lambda_2}]^{\Lambda}$. The transposed annihilation operator $\tilde{a}^{\lambda}_{m} = (-1)^{\lambda-m} a^{\lambda\dagger}_{-m}$, where $a^{\lambda\dagger}_{-m}$ annihilates the state $|\lambda - m\rangle$. It is assumed that the irreducible tensor operator $W^{\Lambda}(\lambda_1\widetilde{\lambda}_2)$ acts on the irreducible tensor space $\mathcal{H}^{\Lambda}$ if $W^{\Lambda}(\lambda_1\widetilde{\lambda}_2)$ transforms under the G–irreducible matrix representation $D^{\Lambda}(g)$. On the other hand, $\mathcal{H}^{\Lambda}$ may be reducible $\mathcal{H}^{L} \times \mathcal{H}^{S}$ ($\Lambda \equiv LS$ for LS-coupling). Then $W^{LS}(l_1\widetilde{l}_2)$ transforms under both $D^{L}(g)$, $D^{S}(g)$ irreducible matrix representations independently. If, however, $\mathcal{H}^{\Lambda}$ is irreducible, then $\Lambda \equiv J$ (jj-coupling).

Judd [46] demonstrated that the application of a second quantised representation of atomic many-body system appears to be especially comfortable for the group-theoretic classification of the states of equivalent electrons of atom. The key feature is that the products of a^{λ}_{m} and $a^{\widetilde{\lambda}\dagger}_{\widetilde{m}}$ form the Lie algebra A_{N_l-1}, where $N_l = \max N = 4l+2$ is a maximal number of electrons in the shell l^N. This implies that the branching rules for the states of l^N are to be obtained. For LS-coupling, the typical reduction scheme reads $\mathrm{U}(N_l) \to \mathrm{Sp}(N_l) \to \mathrm{SO}^{L}(3) \times \mathrm{SU}^{S}(2)$. Particularly, the multiplicities of $\mathrm{Sp}(N_l)$–irreducible representations determine the so-called seniority quantum number v, first introduced by Racah [9, Sec. 6-2]. In this case, it is convenient to form the tensor operators $W^{\kappa\lambda}(\lambda_1\lambda_2) = [a^{\frac{1}{2}\lambda_1} \times a^{\frac{1}{2}\lambda_2}]^{\kappa\lambda}$ on $\mathcal{H}^{q} \equiv \mathcal{H}^{Q} \times \mathcal{H}^{\Lambda}$, where $\mathcal{H}^{Q}$ denotes the quasispin space. The quasispin quantum number Q relates to v by $Q = ([\lambda] - 2v)/4$. Various useful properties of operators on $\mathcal{H}^{q}$ were studied by Rudzikas et. al. [50]. However, starting from f^3 electrons, the last scheme is insufficient and thus additional characteristic numbers are necessary. The complete classification of terms of d^N and f^N configurations was tabulated by Wybourne et. al. [68, 69].

In order to write the Hamiltonian $\widehat{H}$ that describes a system with variable particle number, it is sufficient to express $\widehat{H}$ by its matrix elements as follows

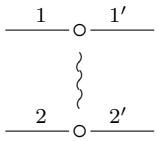
$$\widehat{H} = \widehat{H}_0 + \widehat{V}, \quad \widehat{H}_0 = \sum_{\alpha_1} \widehat{O}_1(\alpha\alpha)\varepsilon_{\alpha_1}, \quad \widehat{V} = \sum_{n=0}^{f} \widehat{V}_n, \quad \widehat{V}_n = F_n[v], \tag{2.40}$$

$$F_n[v] \stackrel{\text{def}}{=} \sum_{I_n(\alpha\bar{\beta})} \widehat{O}_n(\alpha\bar{\beta}) v_n(\alpha\bar{\beta}), \tag{2.41}$$

$$\widehat{O}_n(\alpha\bar{\beta}) \stackrel{\text{def}}{=} :a_{\alpha_1} a_{\alpha_2} \dots a_{\alpha_{n-1}} a_{\alpha_n} a^{\dagger}_{\bar{\beta}_n} a^{\dagger}_{\bar{\beta}_{n-1}} \dots a^{\dagger}_{\bar{\beta}_2} a^{\dagger}_{\bar{\beta}_1}:, \quad \widehat{O}_0(\alpha\bar{\beta}) = 1, \tag{2.42}$$

$$v_n(\alpha\bar{\beta}) \stackrel{\text{def}}{=} v_{\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\bar{\beta}_1\bar{\beta}_2\dots\bar{\beta}_{n-1}\bar{\beta}_n} = \langle \alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n | h(n) | \bar{\beta}_1\bar{\beta}_2\dots\bar{\beta}_{n-1}\bar{\beta}_n \rangle, \tag{2.43}$$

where $I_n(\alpha\bar{\beta}) = \{\alpha_1, \alpha_2, \dots, \alpha_{n-1}, \alpha_n, \bar{\beta}_1, \bar{\beta}_2, \dots, \bar{\beta}_{n-1}, \bar{\beta}_n\}$ is the set of numbers α_i and $\bar{\beta}_j$ $\forall i, j = 1, 2, \dots, n$ that characterise the states $|x_i\rangle = a_{x_i}|0\rangle$, where $x_i = \alpha_i, \bar{\beta}_i$ and $a_{x_i} \equiv a^{\lambda_{x_i}}_{m_{x_i}}$. By default, it is assumed that each operator a_{x_i} is additionally characterised by the principal quantum number n_{x_i}. The notation : : denotes the normal order (or normal form). The operators $h(n)$ with the eigenvalues ε_{x_i} represent the Hamiltonians that are particular for the single particles. Their sum forms the total Hamiltonian H. For the atomic case, see Eq. (2.1). The number f depends on the concrete many-body system. For the atoms and ions, $f = 2$, as all interaction operators $h(n)$ used in atomic spectroscopy are obtained from the Feynman diagram



which requires effort to demonstrate that the path integral is determined in terms of the interaction $\big(1-(\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\big)\exp\big[\mathrm{i}|\varepsilon_1-\varepsilon_{1'}|r_{12}\big]/r_{12}$, where $\boldsymbol{\alpha}_i=\left(\begin{smallmatrix}0 & \boldsymbol{\sigma}_i\\ \boldsymbol{\sigma}_i & 0\end{smallmatrix}\right)$ are the Dirac matrices and $\boldsymbol{\sigma}_i$ denote the 2×2 Pauli matrices. Thus the matrix element of the latter interaction operator on the basis of Dirac 4–spinors results to the sum of Coulomb interaction $1/r_{12}$ and the Breit interaction which particularly is expressed in relativistic and nonrelativistic forms [52, Secs. 1.3, 2.2].

It can be readily checked that the matrix elements of N–electron Hamiltonians H and $\widehat{H}$ on the corresponding basis $\Phi(\Gamma\Pi\Lambda M)$ or else $|\Gamma\Pi\Lambda M\rangle$ are equal. However, $\widehat{H}$ has the eigenstates for all N, while H only for a specified N. According to Kutzelnigg [31, 70], $\widehat{H}$ is called the Fock space Hamiltonian.

2.3.1 Orthogonal subspaces

The task to find the set $X\equiv\{|\Psi_i\rangle\}_{i=1}^{\infty}$ of eigenfunctions of $\widehat{H}$ (see Eq. (2.2)) is found to be partially solvable by using the partitioning technique, first introduced by Feshbach [71]. Later, it was demonstrated by Lindgren et. al. [34] that the present approximation leads to the effective operator approach. In their used formalism, on the other hand, Lindgren and the authors behind [36, 38] commonly regarded the matrix representation of tensor operators. This, however, is a more comfortable representation for practical applications, though it is less universal. The significant opportunities of the irreducible tensor operator techniques in the many-body perturbation theory (MBPT) were demonstrated in Refs. [54, 55, 72, 73].

To find a subset $Y\equiv\{|\Psi_j\rangle\}_{j=1}^{d}\subset X$ of functions $|\Psi_j\rangle$ (with $d<\infty$), the following space partitioning procedure is performed.

2.3.1 Definition. A subset $\widetilde{Y}\equiv\{|\Phi_k\rangle\}_{k=1}^{d}\subset\widetilde{X}\equiv\{|\Phi_p\rangle\}_{p=1}^{\infty}$ satisfies:

(a) the configuration parity $\Pi_k\equiv\Pi^{\widetilde{Y}}\ \forall k=1,2,\ldots,d$ is a constant for all N_k–electron configuration state functions $|\Phi_k\rangle\equiv|\Phi_k^{\widetilde{Y}}\rangle\equiv|\Gamma_k\Pi^{\widetilde{Y}}\Lambda_k M_k\rangle\in\widetilde{Y}$;

(b) the eigenstates $|\Phi_k^{\widetilde{Y}}\rangle$ of $\widehat{H}_0$ contain the configurations of two types:

(1) fully occupied $l_{kt}^{N_{l_{kt}}}$ configurations that particularly determine either core (c) or valence (v) orbitals; the core orbitals are present in all $|\Phi_k^{\widetilde{Y}}\rangle$ for all integers $t<u_k^c$ and for all k, where u_k^c is the number of closed shells in $|\Phi_k^{\widetilde{Y}}\rangle$; the valence orbitals are present in some of the functions $|\Phi_k^{\widetilde{Y}}\rangle$;

(2) partially occupied $l_{kz}^{N_{kz}}$ configurations that determine valence (v) orbitals for all integers $z\le u_k^o$, where u_k^o is the number of open shells in $|\Phi_k^{\widetilde{Y}}\rangle$;

(c) the subset $\widetilde{Y}$ is complete by means of the allocation of valence electrons in all possible ways.

Several meaningful conclusions immediately follow from the definition of $\widetilde{Y}$.

1. The number N_k of electrons in $|\Phi_k^{\widetilde{Y}}\rangle$ equals to

$$N_k=N_k^c+N_k^o,\quad N_k^c=\sum_{t=1}^{u_k^c}N_{l_{kt}}=2\left(u_k^c+2\sum_{t=1}^{u_k^c}l_{kt}\right),\quad N_k^o=\sum_{z=1}^{u_k^o}N_{kz},\tag{2.44}$$

where N_k^c and N_k^o denote the electron occupation numbers in closed and open shells.

2. The subset $\widetilde{Y}$ is partitioned into several subsets $\widetilde{Y}_n$, each of them defined by

$$\widetilde{Y} = \bigcup_{n=1}^{A} \widetilde{Y}_n, \quad \widetilde{Y}_n \stackrel{\text{def}}{=} \{|\Phi_{k_n}^{\widetilde{Y}}\rangle\}_{k_n=d_{n-1}+1}^{d_n}, \quad d_0 = 0, \quad d_A = d. \tag{2.45}$$

The subsets $\widetilde{Y}_n$ are assumed to contain the $\mathcal{N}_n$–electron basis functions $|\Phi_{k_n}^{\widetilde{Y}}\rangle$, where the identities $\mathcal{N}_n \equiv N_{d_{n-1}+1} = N_{d_{n-1}+2} = \ldots = N_{d_n}$ and $\mathcal{N}_1 \neq \mathcal{N}_2 \neq \ldots \neq \mathcal{N}_A$ hold true. This implies that $\widehat{H}_0$ has the eigenstates $\forall\ |\Phi_{k_n}^{\widetilde{Y}}\rangle \in \widetilde{Y}_n$, $\forall n = 1, 2, \ldots, A$, while H_0 has the eigenstates $|\Phi_{k_n}^{\widetilde{Y}}\rangle$ for which $\delta_{N\mathcal{N}_n} \neq 0$. Thus only one specified subset $\widetilde{Y}_n$ fits the eigenvalue equation of H_0. It is found to be the subset $\widetilde{Y}_{\widetilde{n}}$ with $\mathcal{N}_{\widetilde{n}} = N$.

3. Items (a), (c) in Definition 2.3.1 stipulate that the subset $\widetilde{Z} \equiv \widetilde{X} \backslash \widetilde{Y} = \{|\Theta_l\rangle\}_{l=1}^{\infty}$ formed from the functions $|\Theta_l\rangle \equiv |\Phi_{d+l}\rangle$ represents the orthogonal complement of $\widetilde{Y}$. That is, $\widetilde{Y} \cap \widetilde{Z} = \emptyset$. The single-electron orbitals that form the configurations in $|\Theta_l\rangle$ will be called excited (e) or virtual orbitals. These orbitals are absent in $\widetilde{Y}$.

The conclusions in items 1, 3 agree with those inferred by Lindgren [34, Sec. 9.4, p. 199], who used to exploit the traditional Hilbert space approach. On the other hand, item 2 extends this approach to the systems of variable particle number.

Having defined the subsets $\widetilde{Y}, \widetilde{Z} \subset \widetilde{X}$ of vectors of many-body Hilbert spaces, it is sufficient to introduce the subspaces as follows.

2.3.2 Definition. The functions $|\Phi_{k_n}^{\widetilde{Y}}\rangle \in \widetilde{Y}_n$ form the $\mathcal{N}_n$–electron subspace

$$\mathcal{P}_n \stackrel{\text{def}}{=} \Big\{|\Phi_{k_n}^{\widetilde{Y}}\rangle : \langle\Phi_{k_n}^{\widetilde{Y}}|\Phi_{k'_n}^{\widetilde{Y}}\rangle_{\mathcal{H}_n} = \delta_{\Gamma_{k_n}\Gamma_{k'_n}}\delta_{\Lambda_{k_n}\Lambda_{k'_n}}\delta_{M_{k_n}M_{k'_n}} \equiv \delta_{k_n k'_n}, \\ \forall k_n, k'_n = d_{n-1}+1, d_{n-1}+2, \ldots, d_n\Big\} \tag{2.46}$$

of dimension $\dim \mathcal{P}_n = d_n - d_{n-1}$, where $\mathcal{H}_n$ denotes the infinite-dimensional $\mathcal{N}_n$–electron Hilbert space, spanned by all $\mathcal{N}_n$–electron functions $|\Phi_{p_n}\rangle$ from $\widetilde{X}_n \subset \widetilde{X}$.

2.3.3 Corollary. *In accordance with item 2, if $n = \widetilde{n}$, then $\mathcal{H}_{\widetilde{n}} = \mathcal{H}$ denotes the infinite-dimensional N–electron Hilbert space, while $\mathcal{P}_{\widetilde{n}} = \mathcal{P}$ denotes the N–electron subspace of $\mathcal{H}$ with* $\dim \mathcal{P} = d_{\widetilde{n}} - d_{\widetilde{n}-1} \equiv D$.

2.3.4 Corollary. *According to item 3, the orthogonal complement $\mathcal{Q}_n \stackrel{\text{def}}{=} \mathcal{H}_n \ominus \mathcal{P}_n$ of $\mathcal{P}_n$ is spanned by the $\mathcal{N}_n$–electron functions $|\Theta_{l_n}\rangle \in \widetilde{Z}_n \subset \widetilde{Z}$. That is,*

$$\langle\Theta_{l_n}|\Phi_{k_n}^{\widetilde{Y}}\rangle_{\mathcal{H}_n} = 0, \quad \forall l = 1, 2, \ldots, \infty, \quad \forall k = 1, 2, \ldots, d, \quad \forall n = 1, 2, \ldots, A. \tag{2.47}$$

If particularly $n = \widetilde{n}$, then $\mathcal{Q}_{\widetilde{n}} = \mathcal{Q}$ denotes the orthogonal complement of $\mathcal{P}$.

2.3.5 Definition. The functions $|\Phi_k^{\widetilde{Y}}\rangle \in \widetilde{Y}$ form the subspace

$$\mathcal{W} \stackrel{\text{def}}{=} \Big\{|\Phi_k^{\widetilde{Y}}\rangle : \langle\Phi_k^{\widetilde{Y}}|\Phi_{k'}^{\widetilde{Y}}\rangle_{\mathcal{F}} = \sum_{n=1}^{A}\langle\Phi_{k_n}^{\widetilde{Y}}|\Phi_{k'_n}^{\widetilde{Y}}\rangle_{\mathcal{H}_n} = \delta_{\Gamma_k\Gamma_{k'}}\delta_{\Lambda_k\Lambda_{k'}}\delta_{M_k M_{k'}} \equiv \delta_{kk'}, \\ \forall k, k' = 1, 2, \ldots, d\Big\} = \bigoplus_{n=1}^{A}\mathcal{P}_n \subset \mathcal{F} \stackrel{\text{def}}{=} \bigoplus_{n=1}^{A}\mathcal{H}_n \subset \mathfrak{F}, \tag{2.48}$$

where $\mathfrak{F}$ denotes the Fock space.

2.3.6 Corollary. *The orthogonal complement $\mathcal{U} \stackrel{\text{def}}{=} \mathcal{F} \ominus \mathcal{W}$ of $\mathcal{W}$ is spanned by the functions $|\Theta_l\rangle \in \widetilde{Z}$.*

Having defined the many-electron Hilbert spaces, the following proposition is straightforward.

2.3.7 Proposition. *The form* $\widehat{\mathbf{1}}_n\colon\ \mathcal{H}_n \longrightarrow \mathcal{H}_n$, *expressed by*

$$\widehat{\mathbf{1}}_n = \sum_{p_n=1}^{\infty} |\Phi_{p_n}\rangle\langle\Phi_{p_n}|, \quad |\Phi_{p_n}\rangle \in \widetilde{X}_n, \tag{2.49}$$

is a unit operator on $\mathcal{H}_n$.

Proof. For the basis $|\Phi_{p_n}\rangle$, it is evident that (see Definition 2.3.2)

$$\widehat{\mathbf{1}}_n|\Phi_{p_n}\rangle = \sum_{p'_n} |\Phi_{p'_n}\rangle\langle\Phi_{p'_n}|\Phi_{p_n}\rangle_{\mathcal{H}_n} = |\Phi_{p_n}\rangle.$$

For the linear combinations $|\Psi^M\rangle \equiv \sum_{p_n=1}^{M} c_{p_n}|\Phi_{p_n}\rangle$ with $c_{p_n} \in \mathbb{K} = \mathbb{R}, \mathbb{C}$ this is also readily obtainable. That is, $\widehat{\mathbf{1}}_n|\Psi^M\rangle = \sum_{p_n=1}^{M} c_{p_n}\widehat{\mathbf{1}}_n|\Phi_{p_n}\rangle = |\Psi^M\rangle$. □

2.3.8 Corollary. *The form* $\widehat{\mathbf{1}}\colon\ \mathcal{F} \longrightarrow \mathcal{F}$, *expressed by*

$$\widehat{\mathbf{1}} = \sum_{n=1}^{A} \widehat{\mathbf{1}}_n, \tag{2.50}$$

is a unit operator on $\mathcal{F}$.

Proof. The proof directly follows from Definition 2.3.5 and Proposition 2.3.7, recalling that the functions $|\Phi_p\rangle \in \widetilde{X}$ of $\mathcal{F}$ determine any function from the sets $\widetilde{X}_1, \widetilde{X}_2, \ldots, \widetilde{X}_A$. □

Select another basis $Y \equiv \{|\Psi_j\rangle\}_{j=1}^{d}$ of $\mathcal{W} \subset \mathcal{F}$ which is partitioned into the subsets Y_n of $\mathcal{P}_n \subset \mathcal{H}_n$, defined by $Y_n \stackrel{\text{def}}{=} \{|\Psi_{j_n}\rangle\}_{j_n=d_{n-1}+1}^{d_n}$ with $d_0 = 0$, $d_A = d$ (see Eq. (2.45)). As usually (see Eq. (2.2)), it is assumed that the functions $|\Psi_j\rangle \in Y$ designate the eigenstates of $\widehat{H}$ on $\mathcal{F}$, while the functions $|\Psi_{j_{\widetilde{n}}}\rangle$ designate the eigenstates of H on $\mathcal{H}$. Then it is easy to verify that for any integer $n \leq A$,

$$\widehat{\mathbf{1}}_n|\Psi_{j_n}\rangle = |\Psi_{j_n}\rangle = |\Phi^{\mathcal{P}}_{j_n}\rangle + \widehat{Q}_n|\Psi_{j_n}\rangle, \quad |\Phi^{\mathcal{P}}_{j_n}\rangle \stackrel{\text{def}}{=} \widehat{P}_n|\Psi_{j_n}\rangle, \tag{2.51}$$

$$\widehat{P}_n \stackrel{\text{def}}{=} \sum_{k_n=d_{n-1}+1}^{d_n} |\Phi^{\widetilde{Y}}_{k_n}\rangle\langle\Phi^{\widetilde{Y}}_{k_n}|, \quad \widehat{Q}_n \stackrel{\text{def}}{=} \sum_{l_n=1}^{\infty} |\Theta_{l_n}\rangle\langle\Theta_{l_n}|, \quad \widehat{P}_n + \widehat{Q}_n = \widehat{\mathbf{1}}_n. \tag{2.52}$$

If the operator $\widehat{\Omega}\colon\ \mathcal{P}_n \longrightarrow \mathcal{H}_n$ is defined by $\widehat{\Omega}(n)\widehat{P}_n = \widehat{\mathbf{1}}_n$, then $\widehat{Q}_n = \widehat{\Omega}(n)\widehat{P}_n - \widehat{P}_n$ and

$$|\Psi_{j_n}\rangle = \widehat{\Omega}(n)|\Phi^{\mathcal{P}}_{j_n}\rangle. \tag{2.53}$$

$\widehat{\Omega}(n)$ acts on $\mathcal{H}_n$ and it is called the wave operator [34, Sec. 9.4.2, p. 202, Eq. (9.66)]. This implies that the eigenfunctions $|\Psi_{j_{\widetilde{n}}}\rangle$ of H are generated by the wave operator $\widehat{\Omega}(\widetilde{n}) \equiv \widehat{\Omega}$ on the N–electron Hilbert space $\mathcal{H}$. The functions $|\Phi^{\mathcal{P}}_{j_n}\rangle$ are called the model functions of $\mathcal{P}_n$. It was Lindgren [28, 34] who first proved that the wave operator $\widehat{\Omega}$ satisfies the so-called generalised Bloch equation

$$[\widehat{\Omega}, H_0]\widehat{P} = V\widehat{\Omega}\widehat{P} - \widehat{\Omega}\widehat{P}V\widehat{\Omega}\widehat{P} \tag{2.54}$$

which is obtained from the eigenvalue equations of H_0 and H taking into consideration that $[H_0, \widehat{P}] = 0$, where $\widehat{P} \equiv \widehat{P}_{\widetilde{n}}$ (it is also considered that $\widehat{Q} \equiv \widehat{Q}_{\widetilde{n}}$).

For the systems with variable particle number, the action of $\widehat{\Omega}(n)$ must be extended. This will be done by introducing the Fock space operator (see Eq. (2.41))

$$\widehat{S} \stackrel{\text{def}}{=} \widehat{\mathbf{1}} + \sum_{n=1}^{\infty} \widehat{S}_n, \quad \widehat{S}_n \stackrel{\text{def}}{=} F_n[\omega], \tag{2.55}$$

obtained by expanding the exponential ansatz into Taylor series. The coefficients $\omega_n(\alpha\bar{\beta})$ determine matrix elements of some effective interactions indicating the n-particle effects.

The definition of $\widehat{S}$ in Eq. (2.55) is insufficient for the wave operator on $\mathcal{F}$. According to its terms, the wave operator on $\mathcal{H}_n$ maps the space $\mathcal{P}_n$ to $\mathcal{H}_n$ (see Eq. (2.53)). Consequently, the wave operator on $\mathcal{F}$ should map $\mathcal{W}$ to $\mathcal{F}$. To realise the mapping, write the Fock space operator $\widehat{S}\colon\ \mathcal{W} \longrightarrow \mathcal{F}$ so that

$$\widehat{S}\widehat{\mathscr{P}} = \sum_{n=1}^{A} \widehat{\Omega}(n)\widehat{P}_n = \widehat{\mathbf{1}}, \quad |\Phi_j^{\mathcal{P}}\rangle \stackrel{\text{def}}{=} \widehat{\mathscr{P}}|\Psi_j\rangle = \sum_{n=1}^{A} \widehat{P}_n|\Psi_{j_n}\rangle. \tag{2.56}$$

Therefore it turns out that $\widehat{S}$ determines the wave operator on $\mathcal{F}$. The projection operator $\widehat{\mathscr{P}}$ is self-adjoint and idempotent. This fact allows us to verify without supplementary proof that

$$[\widehat{S}, \widehat{H}_0]\widehat{\mathscr{P}} = \widehat{V}\widehat{S}\widehat{\mathscr{P}} - \widehat{S}\widehat{\mathscr{P}}\widehat{V}\widehat{S}\widehat{\mathscr{P}}, \quad [\widehat{H}_0, \widehat{\mathscr{P}}] = 0. \tag{2.57}$$

Apply Eqs. (2.55)-(2.56) to Eq. (2.57) for $n = \widetilde{n}$. The result reads

$$[\widehat{\Omega}, \widehat{H}_0]\widehat{P} = \widehat{V}\widehat{\Omega}\widehat{P} - \widehat{\Omega}\widehat{P}\widehat{V}\widehat{\Omega}\widehat{P}, \tag{2.58}$$

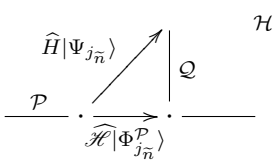
$$\widehat{\Omega} = \widehat{\mathbf{1}}_{\widetilde{n}} + \sum_{n=1}^{\infty} \widehat{\Omega}_n, \quad \widehat{\Omega}_n \stackrel{\text{def}}{=} \widehat{Q}\widehat{S}_n\widehat{P}. \tag{2.59}$$

Eq. (2.58) differs from Eq. (2.54). In Eq. (2.54), the wave operator acts on the N–electron Hilbert space $\mathcal{H}$. In Eq. (2.58), $\widehat{\Omega}$ also acts on $\mathcal{H}$, but in this case, it is represented in terms of $\widehat{S}$ which in turn is projected from $\mathcal{F}$ to $\mathcal{H}$ (see Eq. (2.59)). In other words, Eq. (2.58) designates a second quantised form of the generalised Bloch equation in Eq. (2.54). To compare with, Eq. (2.57) is the Fock space interpretation of the generalised Bloch equation confined on the Hilbert space of specified particle number. On the other hand (see Eq. (2.56)), to solve Eq. (2.57) for $\widehat{S}$, Eq. (2.58) must be solved for $\widehat{\Omega}$.

> The non-variational formulation of the quantum mechanical many-body system appears to be naturally implemented within the frames of the Fock space $\mathfrak{F}$. It is a rather broadened interpretation to compare with the traditional variational approach which is confined to operate on a specified Hilbert space $\mathcal{H}$. The partitioning of the Fock space into its subspaces by the scheme $\mathfrak{F} \supset \mathcal{F} = \mathcal{W} \oplus \mathcal{U}$ makes it possible to consider concurrently the finite-dimensional many-body systems with variable number of particles. In the atomic applications, the procedure of partitioning holds with the ability to account for the effects of ions with different degree of ionisation, as the second quantised Bloch equation handles the effective n-body operators.

2.3.2 Effective operators

The essential advantage of partitioning of N–electron Hilbert space $\mathcal{H}$ into its orthogonal subspaces $\mathcal{P}$, $\mathcal{Q}$ is that the procedure provides an opportunity to define effective operators $\widehat{\mathscr{H}}$ which particularly act on the bounded space, preserving the initially determined integrals of motion, though. In Sec. 2.1, it has been already noted that one of these integrals of motion designates energy of system. The graphical interpretation of the action of effective operators $\widehat{\mathscr{H}}$ on $\mathcal{P}$ can be visualised by the following illustration



(2.60)

where the vector $\widehat{H}|\Psi_{j_{\widetilde{n}}}\rangle$ of $\mathcal{H}$ is projected onto the vector $\widehat{\mathscr{H}}|\Phi^{\mathcal{P}}_{j_{\widetilde{n}}}\rangle$ of $\mathcal{P}$ by the orthogonal projection $\widehat{P}$. Conversely, the vectors $\widehat{H}|\Psi_{j_{\widetilde{n}}}\rangle$, projected by $\widehat{Q}$, lie on the $\mathcal{Q}$ «plane». Making use of Eqs. (2.40), (2.51)-(2.53), it immediately follows that

$$\widehat{\mathscr{H}} = \widehat{P}\widehat{H}\widehat{P} + \widehat{W}, \quad \widehat{W} \stackrel{\text{def}}{=} \sum_{n=1}^{\infty} \widehat{P}(\widehat{V}_1 + \widehat{V}_2)\widehat{\Omega}_n\widehat{P}, \tag{2.61}$$

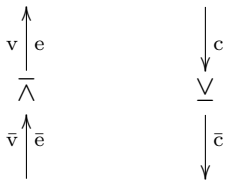
where $\widehat{\Omega}_n$ is of the form presented in Eq. (2.59). Eqs. (2.59), (2.61) point to at least two types of Hilbert space operators: $\widehat{P}\widehat{O}_n(\alpha\bar{\beta})\widehat{P}$ and $\widehat{Q}\widehat{O}_n(\alpha\bar{\beta})\widehat{P}$ (see Eq. (2.42)). To determine their behaviour for a given set $I_n(\alpha\bar{\beta})$ of single-electron orbitals, redefine items (b)(1)-(2), (c), 3 in Sec. 2.3.1 in a more strict manner

$$\begin{array}{ll} \text{(A)} \;\; a_{\mathrm{c}}\widehat{P} = 0, & \text{(C)} \;\; a_{\mathrm{v}}\widehat{P} \neq 0, \\ \text{(B)} \;\; a^{\dagger}_{\bar{\mathrm{e}}}\widehat{P} = 0, & \text{(D)} \;\; a^{\dagger}_{\bar{\mathrm{v}}}\widehat{P} \neq 0. \end{array} \tag{2.62}$$

As already pointed out, items (A)-(B) agree with Ref. [34, Sec. 13.1.2, p. 288, Eq. (13.3)]. Items (C)-(D) embody a mathematical formulation of item (c) in Definition 2.3.1 and are of special significance since they define the so-called complete model space.

The normal orders of products of creation and annihilation operators in $\widehat{O}_n(\alpha\bar{\beta})$ for the specified types (v, e, c) of α, β are these

(2.63)



where $\overline{\wedge}$ (up) and $\underline{\vee}$ (down) denote the direction of electron propagation. For the states created by a_α, write $|\alpha\rangle$. For the states annihilated by $a^{\dagger}_{\bar{\beta}}$, write $|\bar{\beta}\rangle$. Hereafter, the over bar designates annihilated states, but both α and β determine the type of orbital: v, e or c. According to Eq. (2.63), permitted propagations for α and β electrons are to be upwards for $\alpha, \beta = \mathrm{e}, \mathrm{v}$ and downwards for $\alpha, \beta = \mathrm{c}$. In algebraic form of Eq. (2.63), write $:a_\alpha a^{\dagger}_{\bar{\beta}}: = a_\alpha a^{\dagger}_{\bar{\beta}}$ for $\alpha, \beta = \mathrm{v}, \mathrm{e}$ and $:a^{\dagger}_{\bar{\beta}} a_\alpha: = a^{\dagger}_{\bar{\beta}} a_\alpha$ for $\alpha, \beta = \mathrm{c}$.

2.3.9 Lemma. *If $\widehat{O}_n(\alpha\bar{\beta})$ is a Fock space operator and $\widehat{P}$, $\widehat{Q}$ are the orthogonal projections on infinite-dimensional N–electron Hilbert space $\mathcal{H}$, then for any integer $n \leq N$, the following assertions are straightforward:*

i) $\widehat{P}\widehat{O}_n(\alpha\bar{\beta})\widehat{P} \neq 0$ *iff* $\alpha, \beta = \mathrm{v}$;

ii) $\widehat{Q}\widehat{O}_n(\alpha\bar{\beta})\widehat{P} \neq 0$ *iff* $\alpha = \mathrm{v}, \mathrm{e}$ *and* $\beta = \mathrm{v}, \mathrm{c}$;

iii) $\widehat{Q}\widehat{O}_n(\mathrm{v}\bar{\mathrm{v}})\widehat{P} = 0$ *iff* $\sum_{i=1}^{n}(l_{\mathrm{v}_i} + l_{\bar{\mathrm{v}}_i}) \in 2\mathbb{Z}^{+}$.

Observing that self-adjoint operator $\widehat{O}^{\dagger}_n(\alpha\bar{\beta}) = \widehat{O}_n(\bar{\beta}\alpha)$, the following statements are true if Lemma 2.3.9 is valid.

2.3.10 Corollary. *The operator $\widehat{P}\widehat{O}_n(\alpha\bar{\beta})\widehat{Q} \neq 0$ iff $\alpha = \mathrm{v}, \mathrm{c}$ and $\beta = \mathrm{v}, \mathrm{e}$.*

2.3.11 Corollary. *The operator $\widehat{P}\widehat{O}_n(\mathrm{v}\bar{\mathrm{v}})\widehat{Q} = 0$ iff $\sum_{i=1}^{n}(l_{\mathrm{v}_i} + l_{\bar{\mathrm{v}}_i}) \in 2\mathbb{Z}^{+}$.*

Corollaries 2.3.10-2.3.11 are to be proved simply replacing α with β in Lemma 2.3.9.

Proof of Lemma 2.3.9. To prove the lemma, start with item i) which is easy to confirm by passing to Eq. (2.62). To prove item ii), write:

1. $\widehat{Q}a_{\mathrm{v}}\widehat{P} = a_{\mathrm{v}}\widehat{P} - \widehat{P}a_{\mathrm{v}}\widehat{P} \neq 0$ due to items (C)-(D), i).
2. $\widehat{Q}a^{\dagger}_{\bar{\mathrm{v}}}\widehat{P} = a^{\dagger}_{\bar{\mathrm{v}}}\widehat{P} - \widehat{P}a^{\dagger}_{\bar{\mathrm{v}}}\widehat{P} \neq 0$ due to items (C)-(D), i).

3. $\widehat{Q}a_{\rm e}\widehat{P} = a_{\rm e}\widehat{P} - \widehat{P}a_{\rm e}\widehat{P} = a_{\rm e}\widehat{P} = a_{\rm e} - a_{\rm e}\widehat{Q} \neq 0$ due to item i) and Corollary 2.3.4.
4. $\widehat{Q}a^{\dagger}_{\bar{\rm e}}\widehat{P} = a^{\dagger}_{\bar{\rm e}}\widehat{P} - \widehat{P}a^{\dagger}_{\bar{\rm e}}\widehat{P} = 0$ due to items (B), i).
5. $\widehat{Q}a_{\rm c}\widehat{P} = a_{\rm c}\widehat{P} - \widehat{P}a_{\rm c}\widehat{P} = 0$ due to items (A), i).
6. $\widehat{Q}a^{\dagger}_{\bar{\rm c}}\widehat{P} = a^{\dagger}_{\bar{\rm c}}\widehat{P} - \widehat{P}a^{\dagger}_{\bar{\rm c}}\widehat{P} = a^{\dagger}_{\bar{\rm c}}\widehat{P} \neq 0$ due to item i).

To prove item iii), write $|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle$ in an explicit form as follows (see Definition 2.3.1)

$$|l^{N_{k_{\widetilde{n}}1}}_{k_{\widetilde{n}}1} l^{N_{k_{\widetilde{n}}2}}_{k_{\widetilde{n}}2} \ldots l^{N_{k_{\widetilde{n}}\,r-1}}_{k_{\widetilde{n}}\,r-1} l^{N_{k_{\widetilde{n}}r}}_{k_{\widetilde{n}}r} l^{N_{k_{\widetilde{n}}\,r+1}}_{k_{\widetilde{n}}\,r+1} \ldots l^{N_{k_{\widetilde{n}}u_{k_{\widetilde{n}}}}}_{k_{\widetilde{n}}u_{k_{\widetilde{n}}}} \Gamma_{k_{\widetilde{n}}} \Pi^{\widetilde{Y}} \Lambda_{k_{\widetilde{n}}} M_{k_{\widetilde{n}}}\rangle,$$

where $u_{k_{\widetilde{n}}} = u^{c}_{k_{\widetilde{n}}} + u^{o}_{k_{\widetilde{n}}}$. Start from $n = 0$. This is a trivial case, as $\widehat{O}_0(\alpha\bar{\beta}) = 1$ and $\widehat{Q}\widehat{P} = 0$. Suppose $n = 1$. Then

$$\widehat{Q}a_{\rm v_1}a^{\dagger}_{\bar{\rm v}_1}\widehat{P} = \sum_{k_{\widetilde{n}}=d_{\widetilde{n}-1}+1}^{d_{\widetilde{n}}} \sum_{\ell_{\widetilde{n}}=1}^{\infty} |\Theta_{\ell_{\widetilde{n}}}\rangle\langle\Theta_{\ell_{\widetilde{n}}}|\Phi'_{k_{\widetilde{n}}}\rangle_{\mathcal{H}}\langle\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}|. \tag{2.64}$$

The N–electron function $|\Phi'_{k_{\widetilde{n}}}\rangle \equiv a_{\rm v_1}a^{\dagger}_{\bar{\rm v}_1}|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle$ in an explicit form reads

$$\delta(l_{\bar{\rm v}_1}, l_{k_{\widetilde{n}}r})\delta(l_{\rm v_1}, l_{k_{\widetilde{n}}s}) \begin{cases} 0, & N_{k_{\widetilde{n}}s} = 4l_{k_{\widetilde{n}}s} + 2, \\ 1, & \text{otherwise} \end{cases}$$

$$\times\, |l^{N_{k_{\widetilde{n}}1}}_{k_{\widetilde{n}}1} l^{N_{k_{\widetilde{n}}2}}_{k_{\widetilde{n}}2} \ldots l^{N_{k_{\widetilde{n}}\,r-1}}_{k_{\widetilde{n}}\,r-1} l^{N_{k_{\widetilde{n}}r}-1}_{k_{\widetilde{n}}r} l^{N_{k_{\widetilde{n}}\,r+1}}_{k_{\widetilde{n}}\,r+1} \ldots l^{N_{k_{\widetilde{n}}\,s-1}}_{k_{\widetilde{n}}\,s-1} l^{N_{k_{\widetilde{n}}s}+1}_{k_{\widetilde{n}}s} l^{N_{k_{\widetilde{n}}\,s+1}}_{k_{\widetilde{n}}\,s+1} \ldots l^{N_{k_{\widetilde{n}}u_{k_{\widetilde{n}}}}}_{k_{\widetilde{n}}u_{k_{\widetilde{n}}}} \Gamma'_{k_{\widetilde{n}}} \Pi'_{k_{\widetilde{n}}} \Lambda'_{k_{\widetilde{n}}} M'_{k_{\widetilde{n}}}\rangle.$$

In Eq. (2.64), the sum runs over all $k_{\widetilde{n}}$. Consequently, there exists at least one function $|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle$ from the complete set $\widetilde{Y}_{\widetilde{n}}$ such that $l_{\bar{\rm v}_1} = l_{k_{\widetilde{n}}r}$ and $l_{\rm v_1} = l_{k_{\widetilde{n}}s}$ with $N_{k_{\widetilde{n}}s} < 4l_{k_{\widetilde{n}}s} + 2$. Then the parity of obtained non-zero function $|\Phi'_{k_{\widetilde{n}}}\rangle$ equals to $\Pi'_{k_{\widetilde{n}}} = (-1)^{l_{\rm v_1}+l_{\bar{\rm v}_1}}\Pi^{\widetilde{Y}}$. In addition, if $l_{\rm v_1} + l_{\bar{\rm v}_1}$ is even, then $\Pi'_{k_{\widetilde{n}}} = \Pi^{\widetilde{Y}}$ and thus $|\Phi'_{k_{\widetilde{n}}}\rangle$ is equal to $|\Phi^{\widetilde{Y}}_{k'_{\widetilde{n}}}\rangle$ (see item (c) of Definition 2.3.1) up to multiplier, where $k'_{\widetilde{n}}$ acquires any values from $d_{\widetilde{n}-1}+1$ to $d_{\widetilde{n}}$. But $\langle\Theta_{\ell_{\widetilde{n}}}|\Phi^{\widetilde{Y}}_{k'_{\widetilde{n}}}\rangle_{\mathcal{H}} = 0$ due to Corollary 2.3.4.

For $n > 1$, the consideration is consequential and easy to prove. In this case, the parity of $|\Phi'_{k_{\widetilde{n}}}\rangle \equiv \widehat{O}_n(\mathrm{v}\bar{\mathrm{v}})|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle$ equals to $\Pi'_{k_{\widetilde{n}}} = (-1)^{\vartheta_n}\Pi^{\widetilde{Y}}$, where $\vartheta_n = \sum_{i=1}^{n}(l_{\mathrm{v}_i} + l_{\bar{\mathrm{v}}_i})$ assuming that $l_{k_{\widetilde{n}}r_i} = l_{\mathrm{v}_i}$ and $l_{k_{\widetilde{n}}s_i} = l_{\bar{\mathrm{v}}_i}$ for all $i = 1, 2, \ldots, n$ and for all r_i, s_i in the domain of integers $[1, u_{k_{\widetilde{n}}}]$. □

Item iii) of Lemma 2.3.9 may be thought of as an additional parity selection rule whose application to the effective operator approach is of special meaning. The main purpose of the rule is to reject the terms of $\widehat{\Omega}_n$ (see Eq. (2.59)) with zero-valued energy denominators. These energy denominators are obtained from the generalised Bloch equation. Indeed, for the commutator of Eq. (2.58), write

$$\widehat{Q}[\widehat{\Omega}, \widehat{H}_0]\widehat{P} = \sum_{k_{\widetilde{n}}\ell_{\widetilde{n}}} |\Theta_{\ell_{\widetilde{n}}}\rangle\langle\Theta_{\ell_{\widetilde{n}}}|[\widehat{\Omega}, \widehat{H}_0]|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle\langle\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}| = \sum_{n}\sum_{k_{\widetilde{n}}\ell_{\widetilde{n}}} |\Theta_{\ell_{\widetilde{n}}}\rangle\langle\Theta_{\ell_{\widetilde{n}}}|\widehat{\Omega}_n|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle\langle\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}|(\mathscr{E}^{\widetilde{Y}}_{k_{\widetilde{n}}} - \mathscr{E}_{k_{\widetilde{n}}}),$$

where $\mathscr{E}^{\widetilde{Y}}_{k_{\widetilde{n}}}$ and $\mathscr{E}_{k_{\widetilde{n}}}$ denote the eigenvalues of $\widehat{H}_0$ for the eigenfunctions $|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle$ and $|\Theta_{\ell_{\widetilde{n}}}\rangle$, respectively. The right hand side of Eq. (2.58) may be expressed by

$$\sum_{k_{\widetilde{n}}\ell_{\widetilde{n}}} |\Theta_{\ell_{\widetilde{n}}}\rangle\langle\Theta_{\ell_{\widetilde{n}}}|\widehat{\mathscr{V}}|\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}\rangle\langle\Phi^{\widetilde{Y}}_{k_{\widetilde{n}}}|,$$

where the effective operator $\widehat{\mathscr{V}}$ denotes the sum of $F_n[v^{eff}]$ (see Eq. (2.41)) with v^{eff} being some effective interaction. Then

$$\widehat{\Omega}_n = \frac{\widehat{Q}F_n[v^{eff}]\widehat{P}}{\mathscr{E}^{\widetilde{Y}}_{k_{\widetilde{n}}} - \mathscr{E}_{k_{\widetilde{n}}}}.$$

But each eigenvalue $\mathscr{E}^{\widetilde{Y}}_{k_{\tilde{n}}}$, $\mathscr{E}_{k_{\tilde{n}}}$ is the sum of single-electron energies ε_i which are found by solving the single-electron eigenvalue equations for the single-electron eigenstates that correspondingly form $|\Phi^{\widetilde{Y}}_{k_{\tilde{n}}}\rangle$ and $|\Theta_{\ell_{\tilde{n}}}\rangle$. Hence,

$$\widehat{\Omega}_n = \sum_{I_n(\alpha\bar{\beta})} \widehat{Q}\widehat{O}_n(\alpha\bar{\beta})\widehat{P}\omega_n(\alpha\bar{\beta}), \quad \omega_n(\alpha\bar{\beta}) \stackrel{\text{def}}{=} \frac{v_n^{eff}(\alpha\bar{\beta})}{\mathscr{D}_n(\alpha\bar{\beta})}, \quad \mathscr{D}_n(\alpha\bar{\beta}) \stackrel{\text{def}}{=} \sum_{i=1}^{n}(\varepsilon_{\bar{\beta}_i} - \varepsilon_{\alpha_i}), \tag{2.65}$$

where coefficients $\omega_n(\alpha\bar{\beta})$ also characterise the Fock space operator $\widehat{S}$ (see Eq. (2.55)). It immediately follows that for $\alpha = \beta = \mathrm{v}$, the energy denominator $\mathscr{D}_n(\mathrm{v}\bar{\mathrm{v}}) = 0$. Therefore item iii) of Lemma 2.3.9 omits this result for even integers $\sum_{i=1}^{n}(l_{\mathrm{v}_i} + l_{\bar{\mathrm{v}}_i})$.

> The D–dimensional subspace $\mathcal{P}$ of infinite-dimensional N–electron separable Hilbert space $\mathcal{H}$ is formed of the set $\widetilde{Y}_{\tilde{n}}$ of the same parity $\Pi^{\widetilde{Y}}$ configuration state functions $|\Phi^{\widetilde{Y}}_{k_{\tilde{n}}}\rangle$ by allocating the valence electrons in all possible ways (complete model space). In addition, to avoid the divergence of PT terms, the parity selection rule is assumed to be valid. The subspace $\mathcal{P}$ will be called the model space.

The effective operator $\widehat{\mathscr{H}}$ in Eq. (2.61) is usually called the effective Hamiltonian or the effective interaction operator. This is because the eigenvalue equation of Hamiltonian $\widehat{H}$ for $|\Psi_{j_{\tilde{n}}}\rangle$ is found to be partially solved on the model space $\mathcal{P}$ by solving the eigenvalue equation of $\widehat{\mathscr{H}}$ for the model functions $|\Phi^{\mathcal{P}}_{j_{\tilde{n}}}\rangle$ (see Eq. (2.60)).

The second quantised effective operators $\widehat{P}\widehat{H}\widehat{P}$ and $\widehat{\Omega}$ are written in normal order (see Eqs. (2.40)-(2.42), (2.59), (2.61)), while the operator $\widehat{W}$ is not. To «normalise» $\widehat{W}$, the Wick's theorem [40, Eq. (8)] is applied. Then $\widehat{W} = :\widehat{W}: + \sum_{\xi} :\{\widehat{W}\}_{\xi}:$, where the last term denotes the sum of normal-ordered terms with all possible ξ–pair contractions between the m–body part of perturbation $\widehat{V}$ (for $m = 1, 2$) and the n–body part of wave operator $\widehat{\Omega}$ (for $n \in \mathbb{Z}^+$). In this case, $1 \leq \xi \leq \min(2m, 2n)$. In accordance with Lemma 2.3.9, the result $:\widehat{W}: = 0$ is immediate. Thus the operator $\widehat{W}$ in normal order reads

$$\widehat{W} = \sum_{n=1}^{\infty}\sum_{m=1}^{2}\sum_{\xi=1}^{\min(2m,2n)} :\{\widehat{P}\widehat{V}_m\widehat{\Omega}_n\widehat{P}\}_{\xi}: . \tag{2.66}$$

2.3.12 Theorem. *The non-zero terms of effective Hamiltonian $\widehat{\mathscr{H}}$ on the model space $\mathcal{P}$ are generated by a maximum of eight types of the n–body parts of wave operator $\widehat{\Omega}$ with respect to the single-electron states of the set $I_n(\alpha\bar{\beta})$ for all $n \in \mathbb{Z}^+$.*

Proof. The proof is implemented making use of Lemma 2.3.9. The terms of wave operator $\widehat{\Omega}$ that generates $\widehat{\mathscr{H}}$ are drawn in $\widehat{W}$. Therefore it suffices to prove the theorem for the effective operator $\widehat{W}$.

Expand the sums in Eq. (2.66) as follows

$$\widehat{W} = \sum_{\xi,m=1}^{2} :\{\widehat{P}\widehat{V}_m\widehat{\Omega}_1\widehat{P}\}_{\xi}: + \sum_{n=2}^{\infty}\Big(\sum_{\xi=1}^{2} :\{\widehat{P}\widehat{V}_1\widehat{\Omega}_n\widehat{P}\}_{\xi}: + \sum_{\xi=1}^{4} :\{\widehat{P}\widehat{V}_2\widehat{\Omega}_n\widehat{P}\}_{\xi}:\Big).$$

It turns out that for $n = 1$, the following three sets $I_1(\alpha\bar{\beta})$ (see items ii), iii) of Lemma 2.3.9) are valid in Eq. (2.65):

$$I_1^{(1)} \equiv \{\mathrm{e}, \bar{\mathrm{v}}\}, \quad I_1^{(2)} \equiv \{\mathrm{v}, \bar{\mathrm{c}}\}, \quad I_1^{(3)} \equiv \{\mathrm{e}, \bar{\mathrm{c}}\}, \tag{2.67}$$

avoiding for simplicity the subscripts 1 in α_1, $\bar{\beta}_1$.

For $n \geq 2$, the T–body terms of $\widehat{W}$ are derived. Here $T = n-2, n-1, n, n+1$. Particularly, the $(n-2)$–body terms are derived by making the four-pair contractions in $\{\widehat{P}\widehat{V}_2\widehat{\Omega}_n\widehat{P}\}_4$. In

accordance with items ii), iii) of Lemma 2.3.9, it immediately follows that the n–body part of wave operator $\widehat{\Omega}$ must include at least $n-2$ creation and $n-2$ annihilation operators, designating the valence orbitals (item i) of Lemma 2.3.9). Possible sets $I_n(\alpha\bar{\beta})$ of single-electron states that provide non-zero T–body terms are these:

$$I_n^{(1)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_{i-1}, \mathrm{e}, \mathrm{v}_{i+1}, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_n\}, \tag{2.68a}$$

$$I_n^{(2)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_{i-1}, \bar{\mathrm{c}}, \bar{\mathrm{v}}_{i+1}, \ldots, \bar{\mathrm{v}}_n\}, \tag{2.68b}$$

$$I_n^{(3)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_{i-1}, \mathrm{e}, \mathrm{v}_{i+1}, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_{j-1}, \bar{\mathrm{c}}, \bar{\mathrm{v}}_{j+1}, \ldots, \bar{\mathrm{v}}_n\}, \tag{2.68c}$$

$$I_n^{(4)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_{i-1}, \mathrm{e}, \mathrm{v}_{i+1}, \ldots, \mathrm{v}_{j-1}, \mathrm{e}', \mathrm{v}_{j+1}, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_n\}, \tag{2.68d}$$

$$I_n^{(5)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_{i-1}, \bar{\mathrm{c}}, \bar{\mathrm{v}}_{i+1}, \ldots, \bar{\mathrm{v}}_{j-1}, \bar{\mathrm{c}}', \bar{\mathrm{v}}_{j+1}, \ldots, \bar{\mathrm{v}}_n\}, \tag{2.68e}$$

$$I_n^{(6)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_{i-1}, \mathrm{e}, \mathrm{v}_{i+1}, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_{j-1}, \bar{\mathrm{c}}, \bar{\mathrm{v}}_{j+1}, \ldots, \bar{\mathrm{v}}_{k-1}, \bar{\mathrm{c}}', \bar{\mathrm{v}}_{k+1}, \ldots, \bar{\mathrm{v}}_n\}, \tag{2.68f}$$

$$I_n^{(7)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_{i-1}, \mathrm{e}, \mathrm{v}_{i+1}, \ldots, \mathrm{v}_{j-1}, \mathrm{e}', \mathrm{v}_{j+1}, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_{k-1}, \bar{\mathrm{c}}, \bar{\mathrm{v}}_{k+1}, \ldots, \bar{\mathrm{v}}_n\}, \tag{2.68g}$$

$$I_n^{(8)} \equiv \{\mathrm{v}_1, \mathrm{v}_2, \ldots, \mathrm{v}_{i-1}, \mathrm{e}, \mathrm{v}_{i+1}, \ldots, \mathrm{v}_{j-1}, \mathrm{e}', \mathrm{v}_{j+1}, \ldots, \mathrm{v}_n, \bar{\mathrm{v}}_1, \bar{\mathrm{v}}_2, \ldots, \bar{\mathrm{v}}_{k-1}, \bar{\mathrm{c}}, \bar{\mathrm{v}}_{k+1}, \ldots, \bar{\mathrm{v}}_{l-1}, \bar{\mathrm{c}}', \bar{\mathrm{v}}_{l+1}, \ldots, \bar{\mathrm{v}}_n\}. \tag{2.68h}$$

This proves the theorem. □

Theorem 2.3.12 determines that for each fixed Fock space operator $\widehat{S}_n$, there are maximum eight types of the Hilbert space wave operators $\widehat{\Omega}_n$. For example, if the wave function $|\Psi_{j_{\tilde{n}}}\rangle$ distinguishes between single-, two-, three-, four-particle effects ($n = 1, 2, 3, 4$), then Theorem 2.3.12 allows to write $\widehat{\Omega}_n$ as follows

$$\widehat{\Omega}_1 = \sum_{I_1^{(1)}} a_{\mathrm{e}} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\mathrm{e}\bar{\mathrm{v}}} + \sum_{I_1^{(2)}} a_{\mathrm{v}} a^{\dagger}_{\bar{\mathrm{c}}} \omega_{\mathrm{v}\bar{\mathrm{c}}} + \sum_{I_1^{(3)}} a_{\mathrm{e}} a^{\dagger}_{\bar{\mathrm{c}}} \omega_{\mathrm{e}\bar{\mathrm{c}}}, \tag{2.69a}$$

$$\widehat{\Omega}_2 = \sum_{I_2^{(4,5,8)}}{}' a_\alpha a_{\alpha'} a^{\dagger}_{\bar{\beta}'} a^{\dagger}_{\bar{\beta}} \omega_{\alpha\alpha'\bar{\beta}\bar{\beta}'} + \sum_{I_2^{(3)}} a_{\mathrm{e}} a_{\mathrm{v}} a^{\dagger}_{\bar{\mathrm{c}}} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{c}}} + \sum_{I_2^{(1,6)}}{}' a_{\mathrm{e}} a_{\mathrm{v}} a^{\dagger}_{\bar{\beta}'} a^{\dagger}_{\bar{\beta}} \omega_{\mathrm{ev}\bar{\beta}\bar{\beta}'} + \sum_{I_2^{(2,7)}}{}' a_\alpha a_{\alpha'} a^{\dagger}_{\bar{\mathrm{v}}} a^{\dagger}_{\bar{\mathrm{c}}} \omega_{\alpha\alpha'\bar{\mathrm{c}}\bar{\mathrm{v}}}, \tag{2.69b}$$

$$\widehat{\Omega}_3 = \sum_{I_3^{(1,4)}}{}' a_\alpha a_{\alpha'} a_\mu a^{\dagger}_{\bar{\mathrm{v}}''} a^{\dagger}_{\bar{\mathrm{v}}'} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\alpha\alpha'\mu\bar{\mathrm{v}}\bar{\mathrm{v}}'\bar{\mathrm{v}}''} + \sum_{I_3^{(2,5)}}{}' a_{\mathrm{v}} a_{\mathrm{v}'} a_{\mathrm{v}''} a^{\dagger}_{\bar{\mathrm{c}}} a^{\dagger}_{\bar{\beta}'} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\mathrm{vv}'\mathrm{v}''\bar{\mathrm{v}}\bar{\beta}'\bar{\mathrm{c}}} + \sum_{I_3^{(3,6,7,8)}}{}' a_\alpha a_{\alpha'} a_\mu a^{\dagger}_{\bar{\mathrm{c}}} a^{\dagger}_{\bar{\beta}'} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\alpha\alpha'\mu\bar{\mathrm{v}}\bar{\beta}'\bar{\mathrm{c}}}, \tag{2.69c}$$

$$\widehat{\Omega}_4 = \sum_{I_4^{(1,4)}}{}' a_{\mathrm{e}} a_{\alpha'} a_{\mathrm{v}} a_{\mathrm{v}''} a^{\dagger}_{\bar{\mathrm{v}}'''} a^{\dagger}_{\bar{\mathrm{v}}''} a^{\dagger}_{\bar{\mathrm{v}}'} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\mathrm{e}\alpha'\mathrm{vv}''\bar{\mathrm{v}}\bar{\mathrm{v}}'\bar{\mathrm{v}}''\bar{\mathrm{v}}'''} + \sum_{I_4^{(2,5)}}{}' a_{\mathrm{v}} a_{\mathrm{v}'} a_{\mathrm{v}''} a_{\mathrm{v}'''} a^{\dagger}_{\bar{\mathrm{c}}} a^{\dagger}_{\bar{\beta}''} a^{\dagger}_{\bar{\mathrm{v}}'} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\mathrm{vv}'\mathrm{v}''\mathrm{v}'''\bar{\mathrm{v}}\bar{\mathrm{v}}'\bar{\beta}''\bar{\mathrm{c}}} + \sum_{I_4^{(3,6,7,8)}}{}' a_{\mathrm{e}} a_{\alpha'} a_{\mathrm{v}} a_{\mathrm{v}''} a^{\dagger}_{\bar{\mathrm{c}}} a^{\dagger}_{\bar{\beta}''} a^{\dagger}_{\bar{\mathrm{v}}'} a^{\dagger}_{\bar{\mathrm{v}}} \omega_{\mathrm{e}\alpha'\mathrm{vv}''\bar{\mathrm{v}}\bar{\mathrm{v}}'\bar{\beta}''\bar{\mathrm{c}}}, \tag{2.69d}$$

where the single-electron states α_i, $\bar{\beta}_j$ are replaced with α, α', μ, $\bar{\beta}$, e, $\bar{\mathrm{v}}$, etc. Here and elsewhere, it is assumed that the Greek letters denote all three types of single-electron states. The sums with primes denote the following operations

$$\sum_{I_2^{(4,5,8)}}{}' \equiv \sum_{I_2^{(4)}} \delta_{\alpha\mathrm{e}}\delta_{\beta\mathrm{v}} + \sum_{I_2^{(5)}} \delta_{\alpha\mathrm{v}}\delta_{\beta\mathrm{c}} + \sum_{I_2^{(8)}} \delta_{\alpha\mathrm{e}}\delta_{\beta\mathrm{c}}, \tag{2.70a}$$

$$\sum_{I_x^{(a,b)}}{}' \equiv \sum_{I_x^{(a)}} \delta_{\beta\mathrm{v}} + \sum_{I_x^{(b)}} \delta_{\beta\mathrm{c}}, \quad \text{for } x=2, a=1, b=6 \text{ and } x=3,4, a=2, b=5, \tag{2.70b}$$

$$\sum_{I_x^{(a,b)}}{}' \equiv \sum_{I_x^{(a)}} \delta_{\alpha\mathrm{v}} + \sum_{I_x^{(b)}} \delta_{\alpha\mathrm{e}}, \quad \text{for } x=2, a=2, b=7 \text{ and } x=4, a=1, b=4, \tag{2.70c}$$

$$\sum_{I_3^{(1,4)}}{}' \equiv \sum_{I_3^{(1)}} \delta_{\alpha\mathrm{v}}\delta_{\mu\mathrm{e}} + \sum_{I_3^{(4)}} \delta_{\alpha\mathrm{e}}\delta_{\mu\mathrm{v}}, \tag{2.70d}$$

$$\sum_{I_3^{(3,6,7,8)}}{}' \equiv \sum_{I_3^{(3)}} \delta_{\alpha\mathrm{v}}\delta_{\beta\mathrm{v}}\delta_{\mu\mathrm{e}} + \sum_{I_3^{(6)}} \delta_{\alpha\mathrm{v}}\delta_{\beta\mathrm{c}}\delta_{\mu\mathrm{e}} + \sum_{I_3^{(7)}} \delta_{\alpha\mathrm{e}}\delta_{\beta\mathrm{v}}\delta_{\mu\mathrm{v}} + \sum_{I_3^{(8)}} \delta_{\alpha\mathrm{e}}\delta_{\beta\mathrm{c}}\delta_{\mu\mathrm{v}}, \tag{2.70e}$$

$$\sum_{I_4^{(3,6,7,8)}}{}' \equiv \sum_{I_4^{(3)}} \delta_{\alpha\mathrm{v}}\delta_{\beta\mathrm{v}} + \sum_{I_4^{(6)}} \delta_{\alpha\mathrm{v}}\delta_{\beta\mathrm{c}} + \sum_{I_4^{(7)}} \delta_{\alpha\mathrm{e}}\delta_{\beta\mathrm{v}} + \sum_{I_4^{(8)}} \delta_{\alpha\mathrm{e}}\delta_{\beta\mathrm{c}}. \tag{2.70f}$$

For the sake of brevity, in Eqs. (2.70a)-(2.70f) and wherever possible elsewhere, only the types of single-particle orbitals will be designated, but not their values. For instance, in Eq. (2.69b), the term $\sum'_{I_2^{(1,6)}} a_{\mathrm{e}}a_{\mathrm{v}}a^{\dagger}_{\bar{\beta}'}a^{\dagger}_{\bar{\beta}}\omega_{\mathrm{ev}\bar{\beta}\bar{\beta}'}$ contains two two-particle effective matrix elements $\omega_{\mathrm{ev}\bar{\beta}\bar{\beta}'}$ with $\beta=\mathrm{v}$ and $\beta=\mathrm{c}$ (see Eq. (2.70b)). This implies that two single-particle orbitals $\bar{\beta}$ and $\bar{\beta}'$ are of whether valence (v) or core (c) type. That is, the values of orbitals are correspondingly $\bar{\mathrm{v}}$, $\bar{\mathrm{v}}'$ for $\beta=\mathrm{v}$ and $\bar{\mathrm{c}}$, $\bar{\mathrm{c}}'$ for $\beta=\mathrm{c}$.

2.4 Concluding remarks and discussion

For the first time, the method to calculate matrix elements—based on coordinate transformations or else the RCGC technique—has been developed (Sec. 2.2). The technique solves two main tasks. First of all, it reduces the number of multiple integrals of many-electron angular parts up to a single one. Obtained single integral is calculated by introducing the reduced matrix element of founded functions that particularly form the set of $\mathrm{SO}(3)$–irreducible tensor operators (Sec. 2.2.2, Definition 2.2.2, Proposition 2.2.3). Secondly, the technique makes it possible to calculate the matrix elements of irreducible tensor operators on the $\mathrm{SU}(2)$–irreducible matrix representations efficiently. As a result, the method developed here comes down to two distinct lineages, one that can be traced to the basis of separable Hilbert space (Eq. (2.2)), and the other to irreducible matrix representations (Eq. (2.5)) [52, 65, 67].

Sec. 2.3 extends the formulation of many-electron system studied in Sec. 2.1 and Sec. 2.2 to the system with variable particle number. The non-variational or else the perturbative approach to find a finite set of solutions of eigenvalue equation of atomic Hamiltonian has been developed. Based on Feshbach's partitioning technique [71], the generalised Bloch equation [34] has been rewritten in a Fock space approach (Sec. 2.3.1) [39, 70]. As a consequence, proposed algebraic technique based on the effective operator approach (Sec. 2.3.2) leads to meaningful results (Theorem 2.3.12) that directly govern the solutions of generalised Bloch equation as well as the number of terms of effective Hamiltonian (Eq. (2.61)). These results become even more valuable for the higher-order perturbations.

The foremost consequence followed by the suggested Fock space partitioning procedure is that not all computed terms of wave operator (see Eq. (2.59)) attach non-zero contributions to the terms of effective Hamiltonian. This fact, undoubtedly, significantly decreases the amount of computations necessary to find, subsequently, a fixed number of energy levels of atom.

To what has been found in the present section so far, a no less important task is to realise a developed foundation for the effective operators in a second quantised representation. Two major problems take place to solve the task of perturbative expansion for atomic systems. The first one is to solve the generalised Bloch equation for the wave operator on many-electron Hilbert space (see Eqs. (2.58)-(2.59)). The wave operator is listed by the infinite sum of n–body terms. Consequently, for practical computations, it has to be interrupted to a finite number

of terms by excluding the reminder term. The procedure, obviously, leads to approximate values of operator and the wave function as well. Meanwhile, there are also good news. As already pointed out, Theorem 2.3.12 allows us to reduce significantly the number of n–body parts of wave operator. This even more simplifies computations for the approximate wave operator. Blundell et. al. [35] demonstrated that their all-order calculations of energies in cesium with omitted triple and higher-order excitations ($n = 1, 2$) differ from the experimental data at around 1%. In their study for the beryllium-like ions, Safronova et. al. [36] used to exploit the second-order MBPT, clearly demonstrating that their calculations differ from existing experimental data for the nuclear charges ranging from 4 to 100 at the level of $50cm^{-1}$ for triplet states and $500cm^{-1}$ for singlet states. These results obtained by using perturbative methods with relatively low-order excitations are in a smooth agreement with experimental data and thus they strongly motivate for further development of the approach under consideration.

There are two ways to solve the second quantised generalised Bloch equation for the wave operator, one that is to express it by the sum of n–body terms, as in Eq. (2.59), and the other is to express it in terms of the kth–order wave operator, where $k = 1, 2, \ldots$. The first approach is called the coupled-cluster (CC) approximation and the second approach is called the Rayleigh–Schrödinger perturbation theory (RSPT). For the RSPT, the wave operator on N–particle Hilbert space is found to be of the form

$$\widehat{\Omega} = \widehat{\mathbf{1}}_{\tilde{n}} + \sum_{k=1}^{\infty} \widehat{\Omega}^{(k)}, \quad \widehat{\Omega}^{(k)} \stackrel{\text{def}}{=} \sum_{n=1}^{2k} \widehat{\Omega}^{(k)}_{n}. \tag{2.71}$$

To find the kth–order n–body terms $\widehat{\Omega}^{(k)}_{n}$ of wave operator, it is sufficient to express them by Eq. (2.65) replacing the effective matrix elements $\omega_n(\alpha\bar{\beta})$ with the kth–order effective matrix elements $\omega^{(k)}_n(\alpha\bar{\beta})$. For example, if $n = 1, 2, 3, 4$, then $\widehat{\Omega}^{(k)}_{n}$ is given by Eq. (2.69) if ω's are replaced with the corresponding $\omega^{(k)}$'s.

It turns out that it is a fair of choice which form of the solutions of wave operator to be selected, as the mathematical formulation of tensor structure of effective operators remains irrelevant. That is, the difference is in the ω elements only. To find the irreducible tensor form of effective operators such that both – CC and RSPT – approaches could be applicable simply replacing the effective matrix elements, is the second major problem of perturbative formulation, studied here.

To this day, the authors who work in the MBPT usually consider the diagrammatic representation of expansion terms, followed by Goldstone [23] and later by Lindgren et. al. [34]. However, recent works in the higher-order perturbation theory [36, 42, 74, 75] demonstrate, in principal, the inefficiency of such representation, though it is beautiful to behold and efficient in many individual cases. The motivation to develop an algebraic technique suitable for both MBPT approaches is encouraged by the features of nowadays symbolic programming tools as well. The algebraic method that solves the tasks studied in the present section will be developed in thereafter sections.

3 Irreducible tensor operator techniques in atomic spectroscopy

In the present section, the angular reduction schemes of totally antisymmetric tensors $\widehat{O}_n$ (Sec. 2.3, Eq. (2.42)) are studied. The properties of irreducible tensor operators on different tensor spaces and on their tensor products are studied as well. The methods developed here are applicable to both physical operators considered in atomic spectroscopy and effective operators particular to the atomic MBPT. Special attention is paid to the cases $n = 1, 2, 3$, as the contributions of single, double and triple excitations are most valuable for energy corrections observed in MBPT.

The prime issue is the developed technique to reduce a tensor space $\mathcal{H}^{q_1} \times \mathcal{H}^{q_2} \times \ldots \times \mathcal{H}^{q_\ell}$ denoted by $\mathcal{H}_\ell$ to its irreducible subspaces $\mathcal{H}^q$. Irreducible tensor operators on $\mathcal{H}^q$ are classified by the angular reduction schemes that in turn are obtained making use of: the ℓ–numbers for $\ell \in \mathbb{Z}^+$, the irreducible representations $[\lambda]$ of symmetric group S_ℓ, the ℓ_2–tuples, the permutation representations $\widehat{\pi}$ of S_ℓ. To provide suggested technique efficiently, the method of commutative diagrams is originated. The advantage of developed reduction technique to compare with a usual diagrammatic method used in the angular momentum theory is clarified. Namely, it is a convenience to apply it to the systems considered by a large number of momenta or other $\mathrm{SU}(2)$–irreducible representations.

Sec. 3.1 contains a description of a method to classify angular reduction schemes of $\widehat{O}_n$ and establishes the connection between them. In Sec. 3.2, the application to the atomic systems is demonstrated: the irreducible tensor operators are considered when they act on $\ell \leq 6$ electron shells.

3.1 Restriction of tensor space of complex antisymmetric tensors

3.1.1 Classification of angular reduction schemes

To classify reduction schemes, the decomposition of $\widehat{O}_n$ into irreducible tensor series of operators on $\mathcal{H}^q$ is the most convenient choice. In this case, all creation $a_{\alpha_i} \equiv a^{\lambda_i}_{\mu_i}$ and annihilation $a^\dagger_{\bar{\beta}_j} \equiv a^{\lambda_j\dagger}_{\mu_j}$ operators are represented by $a^{\alpha_k}_{\beta_k}$. Also, it makes sense to consider the notation of operator string as follows

$$\widehat{\mathcal{O}}_\ell \stackrel{\text{def}}{=} a^{\alpha_1}_{\beta_1} a^{\alpha_2}_{\beta_2} \ldots a^{\alpha_\ell}_{\beta_\ell}, \quad \alpha_k \equiv {}^1\!/_2\, \lambda_k, \quad \beta_k \equiv {}^{\pm 1}\!/_2\, \mu_k, \tag{3.1}$$

where the irreducible tensor operators a^{α_k} satisfy the following anticommutation rule

$$\left\{a^{\alpha_k}_{\beta_k}, a^{\alpha_l}_{\beta_l}\right\} = (-1)^{\alpha_k - \beta_k + 1} \delta(\alpha_k, \alpha_l) \delta(\beta_k, -\beta_l). \tag{3.2}$$

Then for $\ell \in 2\mathbb{Z}^+$, the ℓ–length string $\widehat{\mathcal{O}}_\ell$ represents $\widehat{O}_{\ell/2}$ on $\mathcal{H}_\ell$ if $\sum_{k=1}^{\ell} \beta_k = \sum_{k=1}^{\ell} \mu_k$. That is, the sum of quasispin basis indices is zero and thus the matrix representation of $\widehat{\mathcal{O}}_\ell$ is diagonal with respect to the particle number. Throughout this text, the last condition is always satisfied for $\ell \in 2\mathbb{Z}^+$, unless explicitly stated otherwise.

A classification of reduction schemes of $\widehat{\mathcal{O}}_\ell$ with $\ell = 2, 3, \ldots, 5$ has been first established by Jucys et. al. [10, Sec. 5-21]. However, only three types of schemes have been considered (A_0, A_1, A_2), concentrating mainly on the permutation properties of angular momentum. In contrast, a general algorithm to classify reduction schemes suitable for $\widehat{\mathcal{O}}_\ell$ with $\ell \in \mathbb{Z}^+$ will be demonstrated here. The schemes will be explicitly listed for $\ell = 2, 3, \ldots, 6$.

To solve the task for ℓ–length string $\widehat{\mathcal{O}}_\ell$, it is convenient to introduce the ℓ–number that contains numerals 1 and 2 only.

3.1.1 Definition. The ℓ–number is a number containing ℓ_2 numerals whose values are 1 and 2 only.

It follows from Definition 3.1.1 that

$$\ell_2 = h_1 + h_2 = \ell - h_2, \tag{3.3}$$

where h_1 and h_2 denote the multiplicities of 1 and 2 in ℓ.

Example. For example, there are two 3–numbers: 12 and 21; $h_1 = h_2 = 1$, $\ell_2 = 2$. On the other hand, number 3 is partitioned by several different ways which, in general, are easily obtained from the tables of irreducible representations (recall «irreps») $[\lambda]$ of symmetric group S_ℓ (see, for example, [76, Appendix 1, p. 261]). In this case, $[\lambda] = [3], [21], [1^3]$. Pick out irreps with the numbers that are present in 3–number. This is $[\lambda] = [21]$. Consequently, the 3–numbers 12 and 21 are to be convenient to characterise them by the S_3–irreducible representation $[21]$; thus they belong to the same conjugacy class $(\alpha) = (1^1 2^2)$ of S_3.

In general, the ℓ–numbers are characterised by the S_ℓ–irreducible representations of the type $[2^{h_2} 1^{h_1}]$. Particularly, if $h_1 = 0$ and $h_2 = 1$, the symmetric S_2–irreducible representation $[2]$ is omitted. Instead of that, the antisymmetric representation $[1^2]$ is chosen.

The example considered above demonstrates that the characterisation of ℓ–numbers by the S_ℓ–irreducible representations is insufficient since both 3–numbers belong to the same class of S_3. Extra characteristics are necessary for a unique labelling of ℓ–numbers. The numbers 12 and 21 differ by the ordering of numerals 1 and 2. Consequently, it is convenient to exploit the properties of ℓ_2–tuple which is an ordered list of ℓ_2 numerals 1, 2. Then 3–numbers are additionally characterised by the two distinct 2–tuples $[[12]]$ and $[[21]]$.

3.1.2 Proposition. *For a fixed $\ell \in \mathbb{Z}^+$, the ℓ–numbers form a set E_ℓ with cardinality*

$$\#E_\ell = \frac{\ell_2!}{h_1! h_2!}, \quad \ell_2 = h_1 + h_2, \tag{3.4}$$

where h_1 and h_2 are the multiplicities of numbers 1 and 2 in the S_ℓ–irreducible representation $[\lambda] \equiv [2^{h_2} 1^{h_1}]$.

Proof. The proof is a simple combinatorial task to find all possible permutations of numbers 1, 2 whose multiplicities are h_1, h_2, where $h_1 + h_2 = \ell_2$. If $h_2 = 1$, there are ℓ_2 ways to permute 2 in ℓ. If $h_2 = 2$, there are $\ell_2(\ell_2 - 1)/2$ ways to permute both 2 numerals in ℓ, etc. For arbitrary h_2, there are $\binom{\ell_2}{h_2}$ ways to permute h_2 numerals 2 in ℓ. □

Still, one more property of ℓ–numbers ought to be determined. It is a connection between two ℓ–numbers with different ℓ. First of all, pick out the $\varkappa$th ℓ–number from the set E_ℓ, where $\varkappa = 1, 2, \ldots, \#E_\ell$. This ℓ–number is uniquely characterised by the S_ℓ–irreducible representation $[\lambda]$ and by the $\ell_2(\varkappa)$–tuple. Secondly, make a change $2 \to 1'$, where a prime over numeral 1 is written to distinguish $1'$ from 1. By doing this, we restricted S_ℓ to its subgroup S_{ℓ_2}. That is, $2 \to 1'$ leads to $\mathrm{S}_\ell \to \mathrm{S}_{\ell'}$, where $\ell' = \ell_2 = \ell - h_2$ (see Eq. (3.3)). Obtained number contains h_1 numerals 1 and h_2 numerals $1'$. The ℓ'–number must be made of it. This is done in the same way as for ℓ–number. Find all $\mathrm{S}_{\ell'}$–irreducible representations $[\lambda'] \equiv [2^{h'_2} 1^{h'_1}]$. Then each $\varkappa'$th ℓ'–number from the set $E_{\ell'}$ is uniquely characterised by the $\mathrm{S}_{\ell'}$–irreducible representation $[\lambda']$ and by the $\ell'_2(\varkappa')$–tuple of length $\ell'_2 = \ell' - h'_2$. Finally, pick out those $\ell'_2(\varkappa')$–tuples which are transformed into the $\ell_2(\varkappa)$–tuple if reversing $1'$ to 2 back again.

Example. Let us go through an example in detail. Assume that the irrep $[\lambda] = [21^2]$. By Proposition 3.1.2, $h_1 = 2$, $h_2 = 1$, $\ell = 4$, $\ell_2 = 3$, $\#E_4 = 3$. This means E_4 contains three 4–numbers characterised by the S_4–irreducible representation $[21^2]$. That is, $E_4 = \{112, 121, 211\}$. Pick out the 1st ($\varkappa = 1$) 4–number 112 which is additionally labelled by the 3(1)–tuple $[[112]]$. Now, make a change $2 \to 1'$ which leads to the restriction $\mathrm{S}_4 \to \mathrm{S}_3$. Obtained number is $11'$. The S_3–irreducible representation of the type $[2^{h'_2} 1^{h'_1}]$ is $[\lambda'] = [21]$. Consequently, $h'_1 = h'_2 = 1$, $\ell'_2 = 2$ and $\#E_3 = 2$. The set $E_3 = \{12, 21\}$, where the 3–numbers 12 ($\varkappa' = 1$) and 21 ($\varkappa' = 2$) are additionally labelled by the 2(1)–tuple $[[12]]$ and by the 2(2)–tuple $[[21]]$, respectively. The numbers 2 in $2(\varkappa')$–tuples are obtained from $11'$ by making the sum $2 = 1 + 1'$ for $\varkappa' = 1$ and the sum $2 = 1 + 1$ for $\varkappa' = 2$. The second sum is excluded since in this case—reversing $1'$ to 2 back again—we get a tuple $[[22]]$ which is absent in E_4. The tuple $[[22]]$ is characteristic for the 4–number that is labelled by the S_4–irreducible representation $[2^2]$. Conversely, the sum $2 = 1 + 1'$ fits the irrep $[21^2]$. Indeed, if $1' \to 2$, then $[[12]] \to [[11']] \to [[112]]$. We write $[[112]] \ltimes [[12]]$ by using the semijoin notation $\ltimes$.

The algorithm considered above is easy to apply to the ℓ–length string $\widehat{\mathcal{O}}_\ell$ for the classification of angular reduction schemes if replacing 1 with α_k and 2 with $\alpha_{kk'}$, where the irreps $\alpha_{kk'}$ are in the Kronecker product $\alpha_k \times \alpha_{k'}$. Then each tuple $t^{[\lambda]}_\varkappa$ characteristic for the $\varkappa$th scheme ($\varkappa$th ℓ–number) obeys the meaning of reduction scheme of $\widehat{\mathcal{O}}_\ell$.

Example. The tuple $[[12]]$ stipulates the scheme $t^{[21]}_1 = (\alpha_1, \alpha_2\alpha_3(\alpha_{23})\alpha)$, where, in general, $\alpha_{12\ldots\ell} \equiv \alpha$.

Tab. 3: Reduction schemes of $\widehat{\mathcal{O}}_{2-5}$

(α)	Tuples	Scheme
(2^1)	$[[2]]$	$\mathscr{T}^{[1^2]}_1$
(1^12^1)	$[[12]]$	$\mathscr{T}^{[21]}_1$
	$[[21]]$	$\mathscr{T}^{[21]}_2$
(2^2)	$[[22]]$	$\mathscr{T}^{[2^2]}_1$
(1^13^1)	$[[211]] \ltimes \mathscr{T}^{[21]}_2$	$\mathscr{T}^{[21^2]}_1$
	$[[121]] \ltimes \mathscr{T}^{[21]}_{2,1}$	$\mathscr{T}^{[21^2]}_{2,3}$
	$[[112]] \ltimes \mathscr{T}^{[21]}_1$	$\mathscr{T}^{[21^2]}_4$
(2^13^1)	$[[221]] \ltimes \mathscr{T}^{[21]}_{2,1}$	$\mathscr{T}^{[2^21]}_{1,2}$
	$[[122]] \ltimes \mathscr{T}^{[21]}_{1,2}$	$\mathscr{T}^{[2^21]}_{3,4}$
	$[[212]] \ltimes \mathscr{T}^{[21]}_{2,1}$	$\mathscr{T}^{[2^21]}_{5,6}$
(1^14^1)	$[[2111]] \ltimes \mathscr{T}^{[21^2]}_1$	$\mathscr{T}^{[21^3]}_1$
	$[[1211]] \ltimes \mathscr{T}^{[21^2]}_{1,3,2}$	$\mathscr{T}^{[21^3]}_{2,3,4}$
	$[[1121]] \ltimes \mathscr{T}^{[21^2]}_{4,2,3}$	$\mathscr{T}^{[21^3]}_{5,6,7}$
	$[[1112]] \ltimes \mathscr{T}^{[21^2]}_4$	$\mathscr{T}^{[21^3]}_8$

Tab. 4: Reduction schemes of $\widehat{\mathcal{O}}_6$

(α)	Tuples	Scheme
(3^2)	$[[222]] \ltimes \mathscr{T}^{[21]}_{2,1}$	$\mathscr{T}^{[2^3]}_{1,2}$
(2^14^1)	$[[2211]] \ltimes \mathscr{T}^{[21^2]}_{1,2,3}$	$\mathscr{T}^{[2^21^2]}_{1,2,3}$
	$[[1221]] \ltimes \mathscr{T}^{[2^2]}_1$	$\mathscr{T}^{[2^21^2]}_4$
	$[[1221]] \ltimes \mathscr{T}^{[21^2]}_{1-4}$	$\mathscr{T}^{[2^21^2]}_{5-8}$
	$[[1122]] \ltimes \mathscr{T}^{[21^2]}_{2,3,4}$	$\mathscr{T}^{[2^21^2]}_{9,10,11}$
	$[[2121]] \ltimes \mathscr{T}^{[2^2]}_1$	$\mathscr{T}^{[2^21^2]}_{12}$
	$[[2121]] \ltimes \mathscr{T}^{[21^2]}_{1-4}$	$\mathscr{T}^{[2^21^2]}_{13-16}$
	$[[2112]] \ltimes \mathscr{T}^{[2^2]}_1$	$\mathscr{T}^{[2^21^2]}_{17}$
	$[[2112]] \ltimes \mathscr{T}^{[21^2]}_{1,4}$	$\mathscr{T}^{[2^21^2]}_{18,19}$
	$[[1212]] \ltimes \mathscr{T}^{[2^2]}_1$	$\mathscr{T}^{[2^21^2]}_{20}$
	$[[1212]] \ltimes \mathscr{T}^{[21^2]}_{1-4}$	$\mathscr{T}^{[2^21^2]}_{21-24}$
(1^15^1)	$[[21111]] \ltimes \mathscr{T}^{[21^3]}_1$	$\mathscr{T}^{[21^4]}_1$
	$[[12111]] \ltimes \mathscr{T}^{[21^3]}_{1-4}$	$\mathscr{T}^{[21^4]}_{2-5}$
	$[[11211]] \ltimes \mathscr{T}^{[21^3]}_{2-7}$	$\mathscr{T}^{[21^4]}_{6-11}$
	$[[11121]] \ltimes \mathscr{T}^{[21^3]}_{5-8}$	$\mathscr{T}^{[21^4]}_{12-15}$
	$[[11112]] \ltimes \mathscr{T}^{[21^3]}_8$	$\mathscr{T}^{[21^4]}_{16}$

Tab. 5: The schemes associated to A_0, A_1, A_2

A_p [a] $\setminus\ \ell$	2	3	4	5	6
A_0	$\mathscr{T}^{[1^2]}_1$	$\mathscr{T}^{[21]}_2$	$\mathscr{T}^{[21^2]}_1$	$\mathscr{T}^{[21^3]}_1$	$\mathscr{T}^{[21^4]}_1$
A_1	$\mathscr{T}^{[1^2]}_1$	$\mathscr{T}^{[21]}_2$	$\mathscr{T}^{[2^2]}_1$	$\mathscr{T}^{[2^21]}_2$	$\mathscr{T}^{[2^21^2]}_3$
A_2	–	–	$\mathscr{T}^{[2^2]}_1$	$\mathscr{T}^{[2^21]}_1$	$\mathscr{T}^{[2^3]}_1$

[a] [10, Sec. 5-21, Eq. (21.12)]

Algorithm. The procedure to classify reduction schemes of $\widehat{\mathcal{O}}_\ell$ is applicable to any ℓ if all other schemes of $\widehat{\mathcal{O}}_{\ell'}$ with $\ell' = 2, 3, \ldots, \ell - 1$ are determined. To perform a task, the following steps should be accomplished.

I. For a given ℓ, make the set E_ℓ of ℓ–numbers (Definition 3.1.1, Proposition 3.1.2) such that each ℓ–number is characterised by the S_ℓ–irreducible representation $[\lambda] \equiv [2^{h_2}1^{h_1}]$ and by the $\ell_2(\varkappa)$–tuple $t^{[\lambda]}_\varkappa$ of length $\ell_2 = \ell - h_2$, where $\varkappa = 1, 2, \ldots, \#E_\ell$ (Eq. (3.4)).

II. Make a restriction $2 \to 1'$ so that $\mathrm{S}_\ell \to \mathrm{S}_{\ell_2}$.

a) If $\ell_2 \leq 3$, then pick out the $\ell_2'(\varkappa')$–tuples $t^{[\lambda']}_{\varkappa'}$ which characterise ℓ_2–numbers labelled by the S_{ℓ_2}–irreducible representations $[\lambda'] \equiv [2^{h_2'}1^{h_1'}]$ and which are transformed into the $\ell_2(\varkappa)$–tuple when reversing $1'$ to 2 back again. Write a correspondence by $t^{[\lambda]}_{\varkappa} \ltimes t^{[\lambda']}_{\varkappa'}$.

b) If $\ell_2 > 3$, repeat the procedure of restriction for S_{ℓ_2} to its subgroup $\mathrm{S}_{\ell_2'}$. If $\ell_2' \leq 3$, then perform item a), otherwise make another restriction $\mathrm{S}_{\ell_2'} \to \mathrm{S}_{\ell_2''}$, etc. At each step of restriction, pick out the tuples that transform to the initial one by making the change $1' \to 2$. Write $t^{[\lambda]}_{\varkappa} \ltimes t^{[\lambda']}_{\varkappa'} \ltimes \ldots \ltimes t^{[\lambda'']}_{\varkappa''}$, where the last tuple is of length $\ell_2'' \leq 3$.

III. Mark off determined $\ell_2(\varkappa)$–tuple $t^{[\lambda]}_{\varkappa}$ expressly by $\mathscr{T}^{[\lambda]}_{\widetilde{\varkappa}} \stackrel{\text{def}}{=} t^{[\lambda]}_{\varkappa} \ltimes t^{[\lambda']}_{\varkappa'} \ltimes \ldots \ltimes t^{[\lambda'']}_{\varkappa''}$, where $\mathscr{T}^{[\lambda]}_{\widetilde{\varkappa}}$ denotes reduction scheme of $\widehat{\mathcal{O}}_\ell$ when the changes $1 \to \alpha_k$ and $2 \to \alpha_{kk'}$ are made. As a result, the semijoin notation obeys its original meaning: the reduction scheme $\mathscr{T}^{[\lambda]}_{\widetilde{\varkappa}}$ of $\widehat{\mathcal{O}}_\ell$ consists of only those reduced Kronecker products which are determined in the reduction scheme $\mathscr{T}^{[\lambda']}_{\varkappa'}$ of $\widehat{\mathcal{O}}_{\ell'}$. The numeration of index $\widetilde{\varkappa}$ is arbitrary. Particularly, $\mathscr{T}^{[\lambda]}_{\widetilde{\varkappa}} = t^{[\lambda]}_{\varkappa}$ if $\ell \leq 3$.

All angular reduction schemes of $\widehat{\mathcal{O}}_\ell$ for $\ell = 1, 2, \ldots, 6$ are listed in Tabs. 3-4, where notations $\mathscr{T}^{[\lambda]}_{a,b,\ldots} = t^{[\lambda]}_{\varkappa} \ltimes \mathscr{T}^{[\lambda]'}_{a',b',\ldots}$ and $\mathscr{T}^{[\lambda]}_{a-b} = t^{[\lambda]}_{\varkappa} \ltimes \mathscr{T}^{[\lambda]'}_{a'-b'}$ signify that $\mathscr{T}^{[\lambda]}_{a} = t^{[\lambda]}_{\varkappa} \ltimes \mathscr{T}^{[\lambda]'}_{a'}$, $\mathscr{T}^{[\lambda]}_{b} = t^{[\lambda]}_{\varkappa} \ltimes \mathscr{T}^{[\lambda]'}_{b'}$, $\mathscr{T}^{[\lambda]}_{a+1} = t^{[\lambda]}_{\varkappa} \ltimes \mathscr{T}^{[\lambda]'}_{a'+1}$, etc. For $\ell = 2, 4, 6$, the operators $\widehat{O}_1$, $\widehat{O}_2$, $\widehat{O}_3$ are reduced according to the schemes: (i) $\mathscr{T}^{[1^2]}_{1}$ for $n = 1$; (ii) $\mathscr{T}^{[2^2]}_{\varkappa}$, $\mathscr{T}^{[21^2]}_{\varkappa'}$ for $n = 2$; (iii) $\mathscr{T}^{[2^3]}_{\varkappa}$, $\mathscr{T}^{[2^21^2]}_{\varkappa'}$, $\mathscr{T}^{[21^4]}_{\varkappa''}$ for $n = 3$.

Reduction schemes $\mathscr{T}^{[\lambda]}_{\varkappa}$ that are related to A_p schemes with $p = 0, 1, 2$ are listed in Tab. 5, where A_2 exists if $\ell \geq 4$. It is clear that Tabs. 3-4 significantly extend the classification presented in Ref. [10].

3.1.2 Correspondence of reduction schemes

Distinct schemes $\mathscr{T}^{[\lambda]}_{\varkappa}$ associated to $\widehat{O}_n$ have been widely studied in several works so far. In Refs. [14, 15], the authors considered schemes $\mathscr{T}^{[1^2]}_{1}$, $\mathscr{T}^{[21]}_{1,2}$, $\mathscr{T}^{[2^2]}_{1}$ which are also widespread in Refs. [54, 55, 77]. This is, however, a case $n = 1, 2$. The schemes $\mathscr{T}^{[2^3]}_{1,2}$, $\mathscr{T}^{[2^21^2]}_{12}$, $\mathscr{T}^{[2^21^2]}_{17}$ associated to $\widehat{O}_3$ have been studied in Refs. [49, 54].

Any scheme $\mathscr{T}^{[\lambda]}_{\varkappa}$ of $\widehat{\mathcal{O}}_\ell$ is linked to another one $\mathscr{T}^{[\lambda']}_{\varkappa'}$ uniquely. To find coefficients that transform one scheme into another, is the main task of the present section. The transformation coefficients for schemes with $\ell = 3, 4, 5$ can be found in [10, Sec. 5]. Therefore the transformation properties of schemes associated to $\widehat{O}_3$ will be studied only.

It can be verified by passing to Tab. 4 that there are in total $42 \cdot 42 = 1,764$ such transformation coefficients for $n = 3$. It can be also easily verified that it suffices to determine 42 coefficients that relate one separate scheme with all the rest, including itself. These coefficients will be called the basis coefficients.

Assume that in any scheme, irreps α_k (see Eq. (3.1)) are listed in the order $\alpha_1, \alpha_2, \ldots, \alpha_6$; irreps in the Kronecker product $\alpha_i \times \alpha_j$ will be labelled by α_{ij}. Expand the operator $\widehat{\mathcal{O}}_6$ on $\mathcal{H}_6$ by the sum of irreducible tensor operators $\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)$ on $\mathcal{H}^q$, where each $\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)$ is associated to reduction scheme $\mathscr{T}^{[\lambda]}_{\varkappa}$. Then

$$\widehat{\mathcal{O}}_6 = \sum_{\alpha\beta} \sum_{\alpha_{\zeta\in\Gamma_\xi}} \widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)\, I([\lambda]\varkappa), \tag{3.5}$$

where the indices $\zeta \in \Gamma_\xi = \{\zeta_1, \zeta_2, \zeta_3, \zeta_4\}$ that label intermediate irreps depend on a specified scheme. The coefficients $I([\lambda]\varkappa)$ are found from the expression

$$\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa) = \sum_{\beta_{i\in\mathcal{I}}} \widehat{\mathcal{O}}_6\, I([\lambda]\varkappa), \quad \mathcal{I} \stackrel{\text{def}}{=} \{1, 2, \ldots, 6\}. \tag{3.6}$$

For example, if $[\lambda]=[2^21^2]$, $\varkappa=12$, then $\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12)$ is associated to the scheme (see Tab. 4) $\mathscr{T}^{[2^21^2]}_{12}=[[2121]]\ltimes[[22]]=\big(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\big)$ and thus

$$\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12)=[[[a^{\alpha_1}\times a^{\alpha_2}]^{\alpha_{12}}\times a^{\alpha_3}]^{\alpha_{123}}\times[[a^{\alpha_4}\times a^{\alpha_5}]^{\alpha_{45}}\times a^{\alpha_6}]^{\alpha_{456}}]^{\alpha}_{\beta}, \tag{3.7}$$

$$I([2^21^2]12)=\sum_{\substack{\beta_{12}\beta_{123}\\ \beta_{45}\beta_{456}}}\langle\alpha_1\beta_1\alpha_2\beta_2|\alpha_{12}\beta_{12}\rangle\langle\alpha_{12}\beta_{12}\alpha_3\beta_3|\alpha_{123}\beta_{123}\rangle\langle\alpha_4\beta_4\alpha_5\beta_5|\alpha_{45}\beta_{45}\rangle \times\langle\alpha_{45}\beta_{45}\alpha_6\beta_6|\alpha_{456}\beta_{456}\rangle\langle\alpha_{123}\beta_{123}\alpha_{456}\beta_{456}|\alpha\beta\rangle. \tag{3.8}$$

3.1.3 Definition. The coefficients ϵ_ξ, $\xi\in\{1,2,\ldots,42\}$ such that

$$\epsilon_\xi\equiv\big(\mathscr{T}^{[2^21^2]}_{12}\big|\mathscr{T}^{[\lambda]}_{\xi}\big)\stackrel{\text{def}}{=}\sum_{\beta_{i\in\mathcal{I}}}I([2^21^2]12)\;I_\xi, \tag{3.9}$$

$$I_\xi\stackrel{\text{def}}{=}\begin{cases} I([2^3]\xi), & \xi=1,2,\\ I([2^21^2]\,\xi-2), & \xi=3,4,\ldots,26,\\ I([21^4]\,\xi-26), & \xi=27,28,\ldots,42\end{cases} \tag{3.10}$$

are called the basis coefficients.

It is easy to verify that there exists a map $\tau_\xi\colon\ \mathscr{T}^{[2^21^2]}_{12}\longrightarrow\mathscr{T}^{[\lambda]}_{\varkappa}$ such that

$$\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)=\sum_{\alpha_{\eta\in\Upsilon\setminus\Upsilon_\xi}}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12)\epsilon_\xi. \tag{3.11}$$

The sum is over all irreps α_η whose indices η are absent in $\mathscr{T}^{[\lambda]}_{\varkappa}$. Υ_ξ is a set of indices of irreps in $\mathscr{T}^{[\lambda]}_{\varkappa}$. Particularly, $\Upsilon_{14}\equiv\Upsilon$. Eq. (3.9) indicates that there exists an inverse map $\tau^{-1}_{\xi'}\colon\ \mathscr{T}^{[\lambda']}_{\varkappa'}\longrightarrow\mathscr{T}^{[2^21^2]}_{12}$. Then the composition $\tau_\xi\circ\tau^{-1}_{\xi'}\colon\ \mathscr{T}^{[\lambda']}_{\varkappa'}\longrightarrow\mathscr{T}^{[\lambda]}_{\varkappa}$ relates two irreducible tensor operators $\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)$ and $\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda']\varkappa')$ by

$$\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)=\sum_{\alpha_{\eta\in\Upsilon_{\xi\xi'}}}\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda']\varkappa')\epsilon_\xi\epsilon_{\xi'},\quad \Upsilon_{\xi\xi'}\stackrel{\text{def}}{=}\big((\Upsilon\setminus\Upsilon_\xi)\bigcup(\Upsilon_{\xi'}\setminus\Upsilon)\big)\setminus\Upsilon_\xi. \tag{3.12}$$

If $\xi=\xi'$, then $\tau_\xi\circ\tau^{-1}_{\xi}=id_{\mathscr{T}^{[\lambda]}_{\varkappa}}$ (identity with respect to operations on irreducible representations in given scheme $\mathscr{T}^{[\lambda]}_{\varkappa}$) and thus

$$\sum_{\alpha_{\eta\in\Upsilon\setminus\Upsilon_\xi}}\epsilon^2_\xi=1. \tag{3.13}$$

Eqs. (3.12)-(3.13) stipulate the following corollary.

3.1.4 Corollary. *The entries*

$$\mathscr{E}_{\xi\xi'}=\mathscr{E}_{\xi'\xi}\stackrel{\text{def}}{=}\sum_{\alpha_{\eta\in\mathcal{M}_{\xi\xi'}}}\epsilon_\xi\epsilon_{\xi'},\quad \mathcal{M}_{\xi\xi'}\stackrel{\text{def}}{=}(\Upsilon\setminus\Upsilon_\xi)\bigcup(\Upsilon\setminus\Upsilon_{\xi'}) \tag{3.14}$$

form a 42×42 *transformation matrix* $\mathscr{E}$ *such that*

$$\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)=\sum_{\alpha_{\eta\in\Upsilon_{\xi'}\setminus\Upsilon_\xi}}\mathscr{E}_{\xi\xi'}\;\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda']\varkappa'). \tag{3.15}$$

It is by no means obvious that $\mathscr{E}_{\xi\,14}=\mathscr{E}_{14\,\xi}=\epsilon_\xi$.

Explicit expressions of ϵ_ξ are to be found exploiting the angular momentum technique based on whether diagrammatic representation followed by Refs. [10, 12] or algebraic manipulations. Here, the algebraic approach actualised by a symbolic programming package *NCoperators* [78] (see also Appendix D) is a preferable one. Obtained expressions are listed in Appendix A.

Definition 3.1.3 indicates that the coefficients ϵ_ξ are basis-independent. Indeed, Eqs. (A.1a)-(A.42a) assert that the basis coefficients are represented by $3nj$–symbols. Specifically $\left\{\begin{smallmatrix} a & b & e \\ d & c & f \end{smallmatrix}\right\}$ denotes $6j$–symbol. Expressions of $12j$–symbols of the second kind (see Eqs. (A.12a), (A.34a), (A.37a), (A.40a)) are determined according to Eq. (19.3) in Ref. [10, Sec. 4-19, p. 102]. The definition of $15j$–symbol of the second kind (see Eq. (A.33a)) is found in Ref. [12, Sec. 4-34, p. 212, Eq. (34.1)]. The triangular deltas $\Delta(a,b,c)$ are encountered due to the orthogonality condition of CGCs.

Operators $\widehat{\mathcal{O}}^{\alpha}([1^2]1)$ associated to the scheme $\mathscr{T}_1^{[1^2]}$ are found to be the building blocks (recall numerals 2 in ℓ–numbers) along with a^{α_k} (numerals 1 in ℓ–numbers) in all other operators $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$. Therefore their properties stipulate the carriage of any operator $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$. The primary and most precious characteristics of $\widehat{\mathcal{O}}^{\alpha}([1^2]1)$ are received from Eq. (3.2). For the sake of clarity, it is useful to alter $\widehat{\mathcal{O}}^{\alpha}([1^2]1)$ by a usual notation $W^{\alpha_{kl}}(\lambda_k\lambda_l)$.

Reduce the Kronecker products $\alpha_k \times \alpha_l$, $\alpha_l \times \alpha_k$ in Eq. (3.2). It requires little effort to find that

$$W^{\alpha_{kl}}_{\beta_{kl}}(\lambda_k\lambda_l) + (-1)^{\alpha_k+\alpha_l+\alpha_{kl}} W^{\alpha_{kl}}_{\beta_{kl}}(\lambda_l\lambda_k) = -[\alpha_k]^{1/2}\delta(\lambda_k,\lambda_l)\delta(\alpha_{kl},0). \tag{3.16}$$

The following results are up front.

$$W^{\alpha_{kl}}(\lambda_k\lambda_l) = (-1)^{\alpha_k+\alpha_l+\alpha_{kl}+1} W^{\alpha_{kl}}(\lambda_l\lambda_k), \quad \lambda_k \neq \lambda_l, \tag{3.17a}$$

$$W^{0}(\lambda_k\lambda_k) = -[\lambda_k]^{1/2}/\sqrt{2}, \tag{3.17b}$$

$$W^{\alpha_{kk}}(\lambda_k\lambda_k) = 0, \quad \alpha_{kk} \in 2\mathbb{Z}^+, \tag{3.17c}$$

$$W^{\alpha_{kk}}(\lambda_k\lambda_k) \neq 0, \quad \alpha_{kk} \in 2\mathbb{Z}^+ + 1. \tag{3.17d}$$

If $W^{\alpha_{kl}}(\lambda_k\lambda_l)$ acts on a tensor space $\mathcal{H}^{Q_{kl}} \times \mathcal{H}^{L_{kl}} \times \mathcal{H}^{S_{kl}}$, then Eq. (3.17) agrees with Eqs. (8.16), (12.39) in Ref. [50]. It is worth to give heed to operators $W^{0\lambda_{kk}}$ and $W^{1\lambda_{kk}}$. The first one is a scalar on $\mathcal{H}^{Q_{kk}}$, while the second is not. In agreement with Eq. (3.17d), $W^{0\lambda_{kk}}$ is non-zero if λ_{kk} is odd; $W^{1\lambda_{kk}}$ is non-zero if λ_{kk} is even. On the other hand, the irreducible tensor operator $W^{\lambda_{kk}}(\lambda_k\lambda_k)$ on $\mathcal{H}^{\Lambda_{kk}}$ is non-zero if only λ_{kk} is even. This is easy to verify from the anticommutation rule $\{a^{\lambda_k}_{\mu_k}, a^{\lambda_l}_{\mu_l}\} = 0$ that holds for creation operators. But $W^{\lambda_{kk}}$ is also a scalar on $\mathcal{H}^{Q_{kk}}$. This immediately implies that the antisymmetric two-electron state characterised by a configuration l_k^2 (in LS-coupling) is generated by $W^{1\lambda_{kk}}$ or $W^{\lambda_{kk}}$ depending on the tensor space under consideration. It is rather not embed by a tensor operator $W^{0\lambda_{kk}}$.

3.1.3 Permutations

The classification of angular reduction schemes $\mathscr{T}_\varkappa^{[\lambda]}$ of $\widehat{\mathcal{O}}_\ell$ is still insufficient. To accomplish the study to its final stage, the basis coefficients (Appendix A) are to be supplemented by the quantities that relate not only reduction schemes but also reduction schemes with somehow permuted irreps within them.

The permutations in schemes are realised through the permutation (reducible) representations $\widehat{\pi}$ or else the permutation operators of S_ℓ [79, Sec. 1.3, p. 9] such that

$$\widehat{\pi}\,\alpha_i = \alpha_{\pi(i)}\ \forall i = 1,2,\ldots,\ell, \quad \pi = \begin{pmatrix} 1 & 2 & \cdots & \ell \\ \pi(1) & \pi(2) & \cdots & \pi(\ell) \end{pmatrix} \in \mathrm{S}_\ell. \tag{3.18}$$

Here and elsewhere, the indices of irreps α_i enumerate operators in a ℓ–length string $\widehat{\mathcal{O}}_\ell$; the values of α_i and α_j with $i \neq j$ can be identical, though (see Sec. 3.1.4).

For $\ell \leq 5$, the permutation properties related to the angular reduction schemes A_0, A_1, A_2 have been considered in Ref. [10]. This is, again, a motive to concentrate on the case $\ell = 6$ only.

The symmetry group S_6 contains $6!$ elements π, each of which is a composition of 2–cycles or else transpositions (ij). For example, $\pi = \left(\begin{smallmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 1 & 2 & 4 & 5 & 6 \end{smallmatrix}\right) = (132)$ is a product of two 2–cycles: $(13)(23)$, $(12)(13)$, $(23)(12)$. It is easy to verify that there are $\ell(\ell-1)/2 = 15$ non-trivial 2–cycles that generate elements π of S_6:

$$\begin{array}{ccccc}(12) & (23) & (34) & (45) & (56)\\ (13) & (24) & (35) & (46) & \\ (14) & (25) & (36) & & \\ (15) & (26) & & & \\ (16) & & & & \end{array} \tag{3.19}$$

To cognise the correspondence of the permutation operator $\widehat{\pi}$ to the associate element $\pi = (ij)$, the notation $\widehat{\pi}_{ij}$ is preferred. For example (see Eq. (3.17a)),

$$\widehat{\pi}_{ij}W^{\alpha_{ij}}(\lambda_i\lambda_j) = W^{\alpha_{ij}}(\lambda_j\lambda_i) = \varpi_{ij}W^{\alpha_{ij}}(\lambda_i\lambda_j), \quad \varpi_{ij} \stackrel{\text{def}}{=} (-1)^{\alpha_i+\alpha_j+\alpha_{ij}+1}. \tag{3.20}$$

Note, Eq. (3.18) indicates that $\widehat{\pi}_{ij}\alpha_{ij} = \alpha_{ji}$. But $|\alpha_i - \alpha_j| \le \alpha_{ij} \le \alpha_i + \alpha_j$ and thus $\alpha_{ij} = \alpha_{ji}$. In general, if there is a map $p_{ij}\colon\ \mathscr{T}_{12}^{[2^21^2]} \longrightarrow (\widehat{\pi}_{ij}\mathscr{T})_{12}^{[2^21^2]}$ such that

$$\widehat{\pi}_{ij}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12) = \sum_{\alpha_{\eta\in\Upsilon\setminus\widehat{\pi}_{ij}\Upsilon}} \varepsilon_{ij}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12), \tag{3.21}$$

then (see Eq. (3.11))

$$\widehat{\pi}_{ij}\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa) = \sum_{\alpha_{\eta\in\mathcal{A}^{ij}_{\xi\xi'}}} \varepsilon_{ij}\epsilon_{\xi'}\epsilon_{(ij)(\xi)}\ \widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda']\varkappa'),\ \epsilon_{(ij)(\xi)} \stackrel{\text{def}}{=} \widehat{\pi}_{ij}\epsilon_{\xi}, \tag{3.22}$$

$$\mathcal{A}^{ij}_{\xi\xi'} \stackrel{\text{def}}{=} \big((\Upsilon\setminus\widehat{\pi}_{ij}\Upsilon)\bigcup(\widehat{\pi}_{ij}(\Upsilon\setminus\Upsilon_{\xi}))\bigcup(\Upsilon_{\xi'}\setminus\Upsilon)\big)\setminus\widehat{\pi}_{ij}\Upsilon_{\xi}, \tag{3.23}$$

where it is assumed that irreps α_i are ordered $(\alpha_1, \alpha_2, \ldots, \alpha_6)$ in $\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda']\varkappa')$, while the ith and jth irreps are permuted in $\widehat{\pi}_{ij}\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa)$. Eq. (3.22) relates two irreducible tensor operators associated to distinct angular reduction schemes ($\mathscr{T}^{[\lambda]}_{\varkappa}$ and $(\widehat{\pi}_{ij}\mathscr{T})^{[\lambda']}_{\varkappa'}$) with the different ordering of irreps within them. The relation is realised through basis coefficients and the recoupling coefficients defined in Eq. (3.21). Eq. (3.22) is easy to generalise for any permutation $(ij)(kl)\ldots(pq)$ by repeating the procedure several times.

Eq. (3.22) is more preferable if rewritten as follows.

3.1.5 Definition. The map $\tau_{\xi}\circ p_{ij}\circ\tau^{-1}_{\xi'}\colon\ \mathscr{T}^{[\lambda']}_{\varkappa'} \longrightarrow (\widehat{\pi}_{ij}\mathscr{T})^{[\lambda]}_{\varkappa}$ is realised through the entries

$$\mathcal{E}^{ij}_{\xi'\xi} = \widehat{\pi}_{ij}\mathcal{E}^{ij}_{\xi\xi'} \stackrel{\text{def}}{=} \sum_{\alpha_{\eta\in\mathcal{N}_{\xi'\xi}}} \varepsilon_{ij}\epsilon_{\xi'}\epsilon_{(ij)(\xi)}, \quad \mathcal{N}_{\xi'\xi} \stackrel{\text{def}}{=} (\Upsilon\setminus\widehat{\pi}_{ij}\Upsilon)\bigcup(\Upsilon\setminus\Upsilon_{\xi'})\bigcup(\widehat{\pi}_{ij}(\Upsilon\setminus\Upsilon_{\xi})) \tag{3.24}$$

of 15 42×42 transformation matrices $\mathcal{E}^{ij}$ so that

$$\widehat{\pi}_{ij}\widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda]\varkappa) = \sum_{\alpha_{\eta\in\Upsilon_{\xi'}\setminus\widehat{\pi}_{ij}\Upsilon_{\xi}}} \mathcal{E}^{ij}_{\xi'\xi}\ \widehat{\mathcal{O}}^{\alpha}_{\beta}([\lambda']\varkappa'). \tag{3.25}$$

3.1.6 Proposition. *The transformation coefficients $\mathscr{E}_{\xi'\xi}$ and $\mathcal{E}^{ij}_{\xi'\xi}$ are related by*

$$\mathscr{E}_{\xi'\xi} = \sum_{\alpha_{\eta\in\mathcal{R}_{\xi''}}} \mathcal{E}^{ij}_{\xi'\xi''}\mathcal{E}^{ij}_{\xi''\xi}, \quad \mathcal{R}_{\xi''} \stackrel{\text{def}}{=} \big((\widehat{\pi}_{ij}\Upsilon_{\xi''})\setminus\Upsilon_{\xi}\big)\bigcup\big((\widehat{\pi}_{ij}\Upsilon_{\xi''})\setminus\Upsilon_{\xi'}\big), \quad \forall i,j\in\mathcal{I}. \tag{3.26}$$

Proof. The most appropriate tool to prove the proposition is the exploitation of map products. First of all, note that $p_{ij}\circ p_{ij} = id_{\mathscr{T}^{[2^21^2]}_{12}}\colon\ \mathscr{T}^{[2^21^2]}_{12} \longrightarrow \mathscr{T}^{[2^21^2]}_{12}$ is an identity in $\mathscr{T}^{[2^21^2]}_{12}$. It is obvious that

$$\tau_{\xi''}\circ p_{ij}\circ\tau^{-1}_{\xi}\circ\tau_{\xi}\circ\tau^{-1}_{\xi'} = \tau_{\xi''}\circ p_{ij}\circ\tau_{\xi'}$$

which can be rewritten by

$$\tau_{\xi'}\circ\tau^{-1}_{\xi} = (\tau_{\xi'}\circ p_{ij}\circ\tau^{-1}_{\xi''})\circ(\tau_{\xi''}\circ p_{ij}\circ\tau^{-1}_{\xi}).$$

According to Corollary 3.1.4 and Definition 3.1.5, the three maps $\tau_{\xi'} \circ \tau_{\xi}^{-1}$, $\tau_{\xi'} \circ p_{ij} \circ \tau_{\xi''}^{-1}$ and $\tau_{\xi''} \circ p_{ij} \circ \tau_{\xi}^{-1}$ are realised through the transformation coefficients $\mathscr{E}_{\xi\xi'}$, $\mathcal{E}^{ij}_{\xi''\xi'}$ and $\mathcal{E}^{ij}_{\xi\xi''}$, respectively. Thus $\mathscr{E}_{\xi\xi'} = \sum \mathcal{E}^{ij}_{\xi\xi''}\mathcal{E}^{ij}_{\xi''\xi'}$. Replacing ξ with ξ' and recalling that $\mathscr{E}_{\xi\xi'} = \mathscr{E}_{\xi'\xi}$, Eq. (3.26) is satisfied. The indices of summation are easily derived subtracting the sets of indices of irreps that are present on both sides of expression. □

3.1.7 Corollary. *If the map* $p_{ij}\colon\ \mathscr{T}_{12}^{[2^21^2]} \longrightarrow (\widehat{\pi}_{ij}\mathscr{T})_{12}^{[2^21^2]}$ *is realised through the coefficient* ε_{ij}*, then*

$$\sum_{\alpha_{\eta\in\Upsilon\setminus\widehat{\pi}_{ij}\Upsilon}} \varepsilon_{ij}^2 = 1. \tag{3.27}$$

Proof. Eq. (3.27) directly follows from the fact that $p_{ij} \circ p_{ij} = id_{\mathscr{T}_{12}^{[2^21^2]}}$. The indices of summation are easily found recalling that (see Definition 3.1.3)

$$1 = \big(\mathscr{T}_{12}^{[2^21^2]}\big|\mathscr{T}_{12}^{[2^21^2]}\big) = \sum_{\alpha_{\eta\in\Upsilon\setminus\widehat{\pi}_{ij}\Upsilon}} \big(\mathscr{T}_{12}^{[2^21^2]}\big|(\widehat{\pi}_{ij}\mathscr{T})_{12}^{[2^21^2]}\big)\big((\widehat{\pi}_{ij}\mathscr{T})_{12}^{[2^21^2]}\big|\mathscr{T}_{12}^{[2^21^2]}\big).$$

□

In agreement with Eq. (3.21), it is useful to generalise Eq. (3.20) by introducing a map $p'_{ij}\colon\ \mathscr{T}_{\varkappa}^{[\lambda]} \longrightarrow (\widehat{\pi}_{ij}\mathscr{T})_{\varkappa}^{[\lambda]}$,

$$\widehat{\pi}_{ij}\widehat{\mathcal{O}}([\lambda]\varkappa) = \varpi_{ij}\widehat{\mathcal{O}}([\lambda]\varkappa) \tag{3.28}$$

which is valid for a specified $[\lambda]$, $\varkappa$, (ij). Then for any operator $\widehat{X}([\lambda]\varkappa)$ associated to the scheme $X_{\varkappa}^{[\lambda]}$ in Tab. 4, the paths τ_{ξ}, τ_{ξ}^{-1}, p_{ij}, p'_{ij} satisfy the following equivalents

$$X_{12}^{[2^21^2]} \xrightarrow{\tau_{\xi}} X_{\varkappa}^{[\lambda]} \equiv \sum_{\alpha_{\eta\in\Upsilon\setminus\Upsilon_{\xi}}} \epsilon_{\xi}\widehat{X}_{\beta}^{\alpha}([2^21^2]12), \tag{3.29a}$$

$$X_{\varkappa}^{[\lambda]} \xrightarrow{\tau_{\xi}^{-1}} X_{12}^{[2^21^2]} \equiv \sum_{\alpha_{\eta\in\Upsilon_{\xi}\setminus\Upsilon}} \epsilon_{\xi}\widehat{X}_{\beta}^{\alpha}([2^21^2]12), \tag{3.29b}$$

$$X_{12}^{[2^21^2]} \xrightarrow{p_{ij}} (\widehat{\pi}_{ij}X)_{12}^{[2^21^2]} \equiv \sum_{\alpha_{\eta\in\Upsilon\setminus\widehat{\pi}_{ij}\Upsilon}} \varepsilon_{ij}\widehat{X}_{\beta}^{\alpha}([2^21^2]12), \tag{3.29c}$$

$$X_{\varkappa}^{[\lambda]} \xrightarrow{p'_{ij}} (\widehat{\pi}_{ij}X)_{\varkappa}^{[\lambda]} \equiv \varpi_{ij}\widehat{X}_{\beta}^{\alpha}([\lambda]\varkappa). \tag{3.29d}$$

Note, X does not necessary represent $\mathscr{T}$. It also fits the quantities $\widehat{\pi}_{ij\ldots l}\mathscr{T}$, $\widehat{\pi}_{ij}\widehat{\pi}_{kl}\ldots\mathscr{T}$, etc. which particularly denote schemes with permuted irreps within them. The same argument folds for operators $\widehat{X}$.

The final task to accomplish the classification of angular reduction schemes of irreducible tensor operators $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ for $\ell = 6$, is to find the transformation coefficients $\mathcal{E}^{ij}_{\xi'\xi}$ (see Definition 3.1.5), as all other coefficients $\mathcal{E}^{\pi}_{\xi'\xi}$ arising duo to permutations of $\widehat{\pi} = \widehat{\pi}_{ij}\ldots\widehat{\pi}_{kl}\widehat{\pi}_{pq}$ are found by applying Eq. (3.25) for several times. To find $\mathcal{E}^{ij}_{\xi'\xi}$, recoupling coefficients ε_{ij} are to be established. By Eq. (3.19), there are 15 recoupling coefficients, each of which is caused by the transposition (ij). The realisation of an assignment by using the traditional method, that is, to recouple Kronecker products of irreps (particularly, angular momenta) of given scheme, is inefficient due to the complexity of schemes. Therefore another method suitable for any ℓ if the basis coefficients are known (see items I-III in Sec. 3.1.1) will be developed.

Algorithm (*Method of commutative diagrams*). The idea is simple: find a commutative diagram

$$\begin{array}{ccccccccc} (\widehat{\pi}_{ij}\mathscr{T})^{[2^21^2]}_{12} & \xleftarrow{\phi_{2s}} & E^{[\lambda_{2s}]}_{\varkappa_{2s}} & \xleftarrow{\phi_{2s-1}} & D^{[\lambda_{2s-1}]}_{\varkappa_{2s-1}} & \xleftarrow{\phi_{2s-2}} & \cdots & \xleftarrow{\phi_{s+1}} & (\widehat{\pi}_{ij}C)^{[\lambda_{s+1}]}_{\varkappa_{s+1}} \\ \uparrow{\scriptstyle p_{ij}} & & & & & & & & \uparrow{\scriptstyle p'_{ij}} \\ \mathscr{T}^{[2^21^2]}_{12} & \xrightarrow{\phi_1} & A^{[\lambda_2]}_{\varkappa_2} & \xrightarrow{\phi_2} & B^{[\lambda_3]}_{\varkappa_3} & \xrightarrow{\phi_3} & \cdots & \xrightarrow{\phi_s} & C^{[\lambda_{s+1}]}_{\varkappa_{s+1}} \end{array} \tag{3.30}$$

such that for a minimal number $\nu_s = 2s+1$ of paths, the composition equals to

$$\phi_{2s} \circ \phi_{2s-1} \circ \ldots \circ \phi_{s+1} \circ p'_{ij} \circ \phi_s \circ \phi_{s-1} \circ \ldots \circ \phi_1 = p_{ij}. \tag{3.31}$$

In Eq. (3.30), $A, B, \ldots, E$ denote angular reduction schemes; the maps ϕ_a depend on specified schemes and they mark off any suitable map τ_ξ, τ_ξ^{-1} or p'_{kl} ($(kl) \neq (ij)$). Eq. (3.30) indicates to find a specified operator $\widehat{C}^\alpha([\lambda_{s+1}]\varkappa_{s+1})$ associated to the scheme $C^{[\lambda_{s+1}]}_{\varkappa_{s+1}}$ such that Eq. (3.28) holds true. Once the operator $\widehat{C}^\alpha([\lambda_{s+1}]\varkappa_{s+1})$ is found, the paths from C to E are easy to perform. Finally, obtained commutative diagram is rewritten in algebraic form by using Eq. (3.29).

The simplest to find are recoupling coefficients ε_{ij} with $j = i+1$ (see the first row in Eq. (3.19)). For all of them, except for $\varepsilon_{12} = \varpi_{12}$, $\varepsilon_{45} = \varpi_{45}$, the commutative diagram reads

$$\begin{array}{ccc} (\widehat{\pi}_{i\,i+1}\mathscr{T})^{[2^21^2]}_{12} & \xleftarrow{\tau_\xi^{-1}} & (\widehat{\pi}_{i\,i+1}\mathscr{T})^{[\lambda]}_{\varkappa} \\ \uparrow{\scriptstyle p_{i\,i+1}} & & \uparrow{\scriptstyle p'_{i\,i+1}} \\ \mathscr{T}^{[2^21^2]}_{12} & \xrightarrow{\tau_\xi} & \mathscr{T}^{[\lambda]}_{\varkappa} \end{array} \tag{3.32}$$

and thus $\nu_s = \nu_1 = 3$, $p_{i\,i+1} = \tau_\xi^{-1} \circ p'_{i\,i+1} \circ \tau_\xi$. This is because $\widehat{\pi}_{i\,i+1}$ permutes any two irreps adjacent to one another within a given scheme. The values of $[\lambda]$, $\varkappa$ and ξ depend on $i \leq 5$. The last step is to write an algebraic expression of given diagram. Start from the path $\tau_\xi\colon\ \mathscr{T}^{[2^21^2]}_{12} \longrightarrow \mathscr{T}^{[\lambda]}_{\varkappa}$. By Eq. (3.29a), write $\sum_{\alpha_{\eta\in\Upsilon\setminus\Upsilon_\xi}} \epsilon_\xi \widehat{\mathcal{O}}^\alpha_\beta([2^21^2]12)$. For the next path $p'_{i\,i+1}\colon\ \mathscr{T}^{[\lambda]}_{\varkappa} \longrightarrow (\widehat{\pi}_{i\,i+1}\mathscr{T})^{[\lambda]}_{\varkappa}$, write (see Eq. (3.29d)) $\sum_{\alpha_{\eta\in\Upsilon\setminus\Upsilon_\xi}} \varpi_{i\,i+1}\epsilon_\xi \widehat{\mathcal{O}}^\alpha_\beta([2^21^2]12)$. Finally, for $\tau_\xi^{-1}\colon\ (\widehat{\pi}_{i\,i+1}\mathscr{T})^{[\lambda]}_{\varkappa} \longrightarrow (\widehat{\pi}_{i\,i+1}\mathscr{T})^{[2^21^2]}_{12}$, write

$$\widehat{\pi}_{i\,i+1}\widehat{\mathcal{O}}^\alpha_\beta([2^21^2]12) = \sum_{\alpha_{\eta\in\mathcal{F}_\xi\setminus\widehat{\pi}_{i\,i+1}\Upsilon}} \varpi_{i\,i+1}\epsilon_\xi\epsilon_{(i\,i+1)(\xi)}\widehat{\mathcal{O}}^\alpha_\beta([2^21^2]12), \tag{3.33}$$

where $\mathcal{F}_\xi \stackrel{\text{def}}{=} (\Upsilon\setminus\Upsilon_\xi)\bigcup(\widehat{\pi}_{i\,i+1}(\Upsilon_\xi\setminus\Upsilon))$. The converse mapping $p_{i\,i+1}\colon\ \mathscr{T}^{[2^21^2]}_{12} \longrightarrow (\widehat{\pi}_{i\,i+1}\mathscr{T})^{[2^21^2]}_{12}$ is realised by Eq. (3.21). Thus both right hand sides of Eqs. (3.21), (3.33) are equal. This implies

$$\varepsilon_{i\,i+1} = \sum_{\alpha_{\eta\in\mathcal{F}_\xi\setminus\Upsilon}} \varpi_{i\,i+1}\epsilon_\xi\epsilon_{(i\,i+1)(\xi)}. \tag{3.34}$$

For $i = 2$, $\xi = 6$; for $i = 3$, $\xi \in \{1, 2, \ldots, 5\}$; for $i = 5$, $\xi = 19$.

The procedure to find commutative diagrams for the rest of ε_{ij} coefficients with indices $j = i+2, i+3, i+4, i+5$ is analogous, except that the diagrams are more complicated. For example, the coefficient ε_{24} is found from the diagram

$$\begin{array}{ccccccccccc} (\widehat{\pi}_{24}\mathscr{T})^{[2^21^2]}_{12} & \xleftarrow{\tau_6^{-1}} & (\widehat{\pi}_{24}\mathscr{T})^{[2^21^2]}_{4} & \xleftarrow{p'_{34}} & (\widehat{\pi}_{234}\mathscr{T})^{[2^21^2]}_{4} & \xleftarrow{\tau_6} & (\widehat{\pi}_{234}\mathscr{T})^{[2^21^2]}_{12} & \xleftarrow{\tau_\xi^{-1}} & (\widehat{\pi}_{234}\mathscr{T})^{[\lambda]}_{\varkappa} \\ \uparrow{\scriptstyle p_{24}} & & & & & & & & \uparrow{\scriptstyle p'_{24}} \\ \mathscr{T}^{[2^21^2]}_{12} & \xrightarrow{\tau_6} & \mathscr{T}^{[2^21^2]}_{4} & \xrightarrow{p'_{23}} & (\widehat{\pi}_{23}\mathscr{T})^{[2^21^2]}_{4} & \xrightarrow{\tau_6^{-1}} & (\widehat{\pi}_{23}\mathscr{T})^{[2^21^2]}_{12} & \xrightarrow{\tau_\xi} & (\widehat{\pi}_{23}\mathscr{T})^{[\lambda]}_{\varkappa} \end{array}$$

which is equivalent for several schemes with $[\lambda]=[2^3]$, $\varkappa=1,2$ and $[\lambda]=[2^21^2]$, $\varkappa=1,2,3$. Then

$$\mathscr{T}_{12}^{[2^21^2]}\xrightarrow{\tau_6}\mathscr{T}_{4}^{[2^21^2]}\equiv\sum_{\alpha_{\eta\in\Upsilon\setminus\Upsilon_6}}\epsilon_6\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),\quad \Upsilon\setminus\Upsilon_6=\{12\},$$

$$\mathscr{T}_{4}^{[2^21^2]}\xrightarrow{p'_{23}}(\widehat{\pi}_{23}\mathscr{T})_{4}^{[2^21^2]}\equiv\sum_{\alpha_{12}}\varpi_{23}\epsilon_6\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

$$(\widehat{\pi}_{23}\mathscr{T})_{4}^{[2^21^2]}\xrightarrow{\tau_6^{-1}}(\widehat{\pi}_{23}\mathscr{T})_{12}^{[2^21^2]}\equiv\sum_{\alpha_{12}}\sum_{\alpha_{\eta\in\widehat{\pi}_{23}(\Upsilon_6\setminus\Upsilon)}}\varpi_{23}\epsilon_6\epsilon_{(23)(6)}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),\quad \Upsilon_6\setminus\Upsilon=\{23\},$$

$$(\widehat{\pi}_{23}\mathscr{T})_{12}^{[2^21^2]}\xrightarrow{\tau_\xi}(\widehat{\pi}_{23}\mathscr{T})_{\varkappa}^{[\lambda]}\equiv\sum_{\alpha_{12}\alpha_{23}}\sum_{\alpha_{\eta\in\widehat{\pi}_{23}(\Upsilon\setminus\Upsilon_\xi)}}\varpi_{23}\epsilon_6\epsilon_{(23)(6)}\epsilon_{(23)(\xi)}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

$$(\widehat{\pi}_{23}\mathscr{T})_{\varkappa}^{[\lambda]}\xrightarrow{p'_{24}}(\widehat{\pi}_{234}\mathscr{T})_{\varkappa}^{[\lambda]}\equiv\sum_{\alpha_{12}\alpha_{23}}\sum_{\alpha_{\eta\in\widehat{\pi}_{23}(\Upsilon\setminus\Upsilon_\xi)}}\varpi_{23}\varpi_{24}\epsilon_6\epsilon_{(23)(6)}\epsilon_{(23)(\xi)}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

$$(\widehat{\pi}_{234}\mathscr{T})_{\varkappa}^{[\lambda]}\xrightarrow{\tau_\xi^{-1}}(\widehat{\pi}_{234}\mathscr{T})_{12}^{[2^21^2]}\equiv\sum_{\alpha_{12}\alpha_{23}}\sum_{\alpha_{\eta\in A_\xi}}\varpi_{23}\varpi_{24}\epsilon_6\epsilon_{(23)(6)}\epsilon_{(23)(\xi)}\epsilon_{(234)(\xi)}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

$$A_\xi\stackrel{\text{def}}{=}\big((\widehat{\pi}_{23}(\Upsilon\setminus\Upsilon_\xi))\bigcup(\widehat{\pi}_{234}(\Upsilon_\xi\setminus\Upsilon))\big),$$

$$(\widehat{\pi}_{234}\mathscr{T})_{12}^{[2^21^2]}\xrightarrow{\tau_6}(\widehat{\pi}_{234}\mathscr{T})_{4}^{[2^21^2]}\equiv\sum_{\alpha_{12}\alpha_{23}}\sum_{\alpha_{\eta\in A_\xi}}\sum_{\alpha_{\eta'\in\widehat{\pi}_{234}(\Upsilon\setminus\Upsilon_6)}}\varpi_{23}\varpi_{24}\epsilon_6\epsilon_{(23)(6)}\epsilon_{(23)(\xi)}\epsilon_{(234)(\xi)}\times\epsilon_{(234)(6)}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

$$(\widehat{\pi}_{234}\mathscr{T})_{4}^{[2^21^2]}\xrightarrow{p'_{34}}(\widehat{\pi}_{24}\mathscr{T})_{4}^{[2^21^2]}\equiv\sum_{\alpha_{12}\alpha_{23}\alpha_{13}}\sum_{\alpha_{\eta\in A_\xi}}\varpi_{23}\varpi_{24}\varpi_{34}\epsilon_6\epsilon_{(23)(6)}\epsilon_{(23)(\xi)}\epsilon_{(234)(\xi)}\times\epsilon_{(234)(6)}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

$$(\widehat{\pi}_{24}\mathscr{T})_{4}^{[2^21^2]}\xrightarrow{\tau_6^{-1}}(\widehat{\pi}_{24}\mathscr{T})_{12}^{[2^21^2]}\equiv\sum_{\alpha_{12}\alpha_{23}\alpha_{13}}\sum_{\alpha_{\eta\in A_\xi}}\sum_{\alpha_{\eta'\in\widehat{\pi}_{24}(\Upsilon_6\setminus\Upsilon)}}\varpi_{23}\varpi_{24}\varpi_{34}\epsilon_6\epsilon_{(23)(6)}\epsilon_{(23)(\xi)}\times\epsilon_{(234)(\xi)}\epsilon_{(234)(6)}\epsilon_{(24)(6)}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12).$$

Thus

$$\varepsilon_{24}=\sum_{\alpha_{13}\alpha_{23}\alpha_{34}}\sum_{\alpha_{\eta\in A_\xi\setminus\Upsilon}}f_{24}\epsilon_6\epsilon_{(23)(6)}\epsilon_{(23)(\xi)}\epsilon_{(234)(\xi)}\epsilon_{(234)(6)}\epsilon_{(24)(6)},\tag{3.35}$$

where the multiplier f_{ij} denotes the following product

$$f_{ij}\stackrel{\text{def}}{=}\prod_{k=1}^{j-i}\prod_{l=1}^{j-i-1}\varpi_{i\,i+k}\,\varpi_{i+l\,j}.\tag{3.36}$$

Other coefficients $\varepsilon_{i\,i+2}$ are found from the commutative diagrams with $\nu_s=\nu_2=5$ so that $p'_{tu}\circ\tau_\xi^{-1}\circ p'_{i\,i+2}\circ\tau_\xi\circ p'_{rs}=p_{i\,i+2}$. A composition is realised for the numbers r, s, t, u such that $\widehat{\pi}_{i\,i+2}=\widehat{\pi}_{tu}\widehat{\pi}_{i\,i+2}\widehat{\pi}_{rs}$. It is to be whether $(rs)=(i\,i+1)$, $(tu)=(i+1\,i+2)$ or $(tu)=(i\,i+1)$, $(rs)=(i+1\,i+2)$. Then

$$\varepsilon_{i\,i+2} = \sum_{\alpha_{\eta\in B_\xi\setminus\Upsilon}} f_{i\,i+2}\epsilon_{(i\,i+1)(\xi)}\epsilon_{(i\,i+1\,i+2)(\xi)}, \quad i=1,4, \tag{3.37}$$

$$B_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{i\,i+1}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{i\,i+1\,i+2}(\Upsilon_\xi\setminus\Upsilon)\big). \tag{3.38}$$

$$\varepsilon_{35} = \sum_{\alpha_{\eta\in B'_\xi\setminus\Upsilon}} f_{35}\epsilon_{(45)(\xi)}\epsilon_{(354)(\xi)}, \tag{3.39}$$

$$B'_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{i+1\,i+2}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{i\,i+2\,i+1}(\Upsilon_\xi\setminus\Upsilon)\big), \quad i=3. \tag{3.40}$$

For $i=1$, $\xi=6$; for $i=3$, $\xi\in\{1,2,\ldots,5\}$; for $i=4$, $\xi=19$.

The coefficients $\varepsilon_{i\,i+3}$ are characterised by the commutative diagrams with $\nu_s=\nu_5=11$ so that

$$p_{14} = p'_{24}\circ\tau_6^{-1}\circ p'_{34}\circ\tau_6\circ\tau_\xi^{-1}\circ p'_{14}\circ\tau_\xi\circ\tau_6^{-1}\circ p'_{13}\circ\tau_6\circ p'_{12}, \quad \xi\in\{1,2,\ldots,5\}, \tag{3.41a}$$

$$p_{25} = p'_{24}\circ\tau_6^{-1}\circ p'_{35}\circ\tau_6\circ\tau_\xi^{-1}\circ p'_{25}\circ\tau_\xi\circ\tau_6^{-1}\circ p'_{23}\circ\tau_6\circ p'_{45}, \quad \xi\in\{1,2,\ldots,5\}, \tag{3.41b}$$

$$p_{36} = \tau_{19}^{-1}\circ p'_{35}\circ\tau_{19}\circ p'_{34}\circ\tau_\xi^{-1}\circ p'_{36}\circ\tau_\xi\circ p'_{46}\circ\tau_{19}^{-1}\circ p'_{56}\circ\tau_{19}, \quad \xi\in\{1,2\}. \tag{3.41c}$$

From these diagrams it follows that

$$\varepsilon_{14} = \sum_{\alpha_{13}\alpha_{23}\alpha_{34}}\sum_{\alpha_{\eta\in C_\xi\setminus\Upsilon}} f_{14}\epsilon_{(12)(6)}\epsilon_{(123)(6)}\epsilon_{(123)(\xi)}\epsilon_{(1234)(\xi)}\epsilon_{(1234)(6)}\epsilon_{(124)(6)}, \tag{3.42a}$$

$$\varepsilon_{25} = \sum_{\alpha_{13}\alpha_{23}\alpha_{35}}\sum_{\alpha_{\eta\in C'_\xi\setminus\Upsilon}} f_{25}\epsilon_{(45)(6)}\epsilon_{(23)(45)(6)}\epsilon_{(23)(45)(\xi)}\epsilon_{(2354)(\xi)}\epsilon_{(2354)(6)}\epsilon_{(254)(6)}, \tag{3.42b}$$

$$\varepsilon_{36} = \sum_{\alpha_{34}\alpha_{35}\alpha_{56}}\sum_{\alpha_{\eta\in C''_\xi\setminus\Upsilon}} f_{36}\epsilon_{19}\epsilon_{(56)(19)}\epsilon_{(465)(\xi)}\epsilon_{(3654)(\xi)}\epsilon_{(365)(19)}\epsilon_{(36)(19)}, \tag{3.42c}$$

where $C_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{123}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{1234}(\Upsilon_\xi\setminus\Upsilon)\big)$, $C'_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{23}\widehat{\pi}_{45}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{2354}(\Upsilon_\xi\setminus\Upsilon)\big)$ and $C''_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{465}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{3654}(\Upsilon_\xi\setminus\Upsilon)\big)$.

The advantage of method of commutative diagrams as a language of combinatorial computation appears to be evident especially in the cases $j=i+4, i+5$. The coefficients ε_{15}, ε_{26}, ε_{16} can be found from the commutative diagrams with $\nu_s=\nu_6=13$ for $j=i+4$ and $\nu_s=\nu_7=15$ for $j=i+5$. That is,

$$p_{15} = p'_{25}\circ p'_{14}\circ\tau_6^{-1}\circ p'_{35}\circ\tau_6\circ\tau_\xi^{-1}\circ p'_{15}\circ\tau_\xi\circ\tau_6^{-1}\circ p'_{45}\circ p'_{13}\circ\tau_6\circ p'_{12}, \tag{3.43a}$$

$$p_{26} = \tau_{22}^{-1}\circ p'_{25}\circ p'_{36}\circ\tau_{22}\circ p'_{24}\circ\tau_\xi^{-1}\circ p'_{26}\circ\tau_\xi\circ p'_{46}\circ\tau_{22}^{-1}\circ p'_{56}\circ p'_{23}\circ\tau_{22}, \tag{3.43b}$$

$$p_{16} = p'_{26}\circ\tau_{22}^{-1}\circ p'_{15}\circ p'_{36}\circ\tau_{22}\circ p'_{14}\circ\tau_\xi^{-1}\circ p'_{16}\circ\tau_\xi\circ p'_{46}\circ\tau_{22}^{-1}\circ p'_{56}\circ p'_{13}\circ\tau_{22}\circ p'_{12}, \tag{3.43c}$$

where $\xi\in\{1,2,\ldots,5\}$. The corresponding coefficients are

$$\varepsilon_{15} = \sum_{\alpha_{13}\alpha_{23}\alpha_{35}}\sum_{\alpha_{\eta\in D_\xi\setminus\Upsilon}} f_{15}\epsilon_{(12)(6)}\epsilon_{(123)(45)(6)}\epsilon_{(123)(45)(\xi)}\epsilon_{(12354)(\xi)}\epsilon_{(12354)(6)}\epsilon_{(1254)(6)}, \tag{3.44a}$$

$$\varepsilon_{26} = \sum_{\substack{\alpha_{13}\alpha_{23}\alpha_{24}\\ \alpha_{25}\alpha_{36}\alpha_{56}}}\sum_{\alpha_{\eta\in D'_\xi\setminus\Upsilon}} f_{26}\epsilon_{22}\epsilon_{(23)(56)(22)}\epsilon_{(23)(465)(\xi)}\epsilon_{(23654)(\xi)}\epsilon_{(2365)(22)}\epsilon_{(26)(22)}, \tag{3.44b}$$

$$\varepsilon_{16} = \sum_{\substack{\alpha_{13}\alpha_{14}\alpha_{15}\\ \alpha_{23}\alpha_{36}\alpha_{56}}}\sum_{\alpha_{\eta\in E_\xi\setminus\Upsilon}} f_{16}\epsilon_{(12)(22)}\epsilon_{(123)(56)(22)}\epsilon_{(123)(465)(\xi)}\epsilon_{(123654)(\xi)}\epsilon_{(12365)(22)}\epsilon_{(126)(22)} \tag{3.44c}$$

with $D_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{123}\widehat{\pi}_{45}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{12354}(\Upsilon_\xi\setminus\Upsilon)\big)$, $D'_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{23}\widehat{\pi}_{465}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{23654}(\Upsilon_\xi\setminus\Upsilon)\big)$ and $E_\xi \stackrel{\text{def}}{=} \big(\widehat{\pi}_{123}\widehat{\pi}_{465}(\Upsilon\setminus\Upsilon_\xi)\big)\bigcup\big(\widehat{\pi}_{123654}(\Upsilon_\xi\setminus\Upsilon)\big)$.

In [80, Tab. 3], the coefficients ε_{26} and ε_{16} have been found to be obtained from the expressions

$$\widehat{\pi}_{26}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12) = \sum_{\alpha_{13}\alpha_{36}} \varpi_{36}\epsilon_{(26)(6)}\epsilon_{(236)(6)}\widehat{\pi}_{23}\widehat{\pi}_{36}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

$$\widehat{\pi}_{26}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12) = \varpi_{16}\widehat{\pi}_{12}\widehat{\pi}_{16}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12).$$

In the language of commutative diagrams, the coefficients ε_{26} and ε_{16} are found from the diagrams with $\nu_s = \nu_8 = 17$ and $\nu_s = \nu_9 = 19$ compositions, respectively. These numbers point to an ocular demonstration of the advantage of diagrammatic method presented here.

To conclude, it is worth to mention that most of commutative diagrams studied in this section can be drawn in several different ways with the same number ν_s. For instance,

$$p_{25} = \tau_6^{-1} \circ p'_{35} \circ \tau_6 \circ p'_{24} \circ \tau_\xi^{-1} \circ p'_{25} \circ \tau_\xi \circ \tau_6^{-1} \circ p'_{45} \circ p'_{23} \circ \tau_6$$

is also a composition of $\nu_s = \nu_5 = 11$ maps, thus it is equivalent to the diagram characterised by the composition presented in Eq. (3.41b). If, for instance, $\phi_i \circ \phi_j = \phi_j \circ \phi_i$, then it ought to be possible to construct the classes C_i that contain equivalent elements $\phi_i = \phi_j^{-1} \circ \phi_i \circ \phi_j$ with all possible j including $j = i$. Such classification is still to be clarified.

3.1.4 Equivalent permutations

In the present section, the following statement will be proved.

3.1.8 Theorem. *Let $\widehat{\pi}$ be a permutation representation of S_ℓ. If the irreducible tensor operator $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ on $\mathcal{H}^q$ contains a set of equal irreducible representations α_s, $s = 1, 2, \ldots, t < \ell$, then there exists a permutation representation $\widehat{\pi}_{\min}$ which represents a cycle of the smallest possible length or a product of cycles of the smallest possible length such that the correspondence*

$$\mathcal{E}^{\pi}_{\xi'\xi} = \mathcal{E}^{\pi_{\min}}_{\xi'\xi} \tag{3.45}$$

is satisfied, though the map $\tau_\xi \circ p_{\pi_{\min}} \circ \tau_{\xi'}^{-1}$: $\mathscr{T}^{[\lambda']}_{\varkappa'} \longrightarrow (\widehat{\pi}_{\min}\mathscr{T})^{[\lambda]}_{\varkappa}$ does not exist.

An incitement to find the smallest possible length $\widehat{\pi}_{\min}$ associated to $\widehat{\pi}$ is caused by a prospect to reduce the number of intermediate irreps that appear due to transformations: the less number of transpositions, the less number of indices of summation.

To avoid further misleading, it is more suitable to label irreps α_s with $s \leq t$ by ς_x, where $x = i, j, k, l, p, q, \ldots$. That is, α_s designates the irrep of the sth operator a^{α_s}; ς_x denotes its value, though.

Suppose there is operator $\widehat{\mathcal{O}}^{\alpha}_{\beta}([21]2)$ associated to the scheme $\mathscr{T}_2^{[21]}$ (see Tab. 3) with irreps $\alpha_1 = \alpha_2 = \varsigma_i$, $\alpha_3 = \varsigma_j$, $\alpha = \varsigma$, $\beta = \iota$. In accordance with Eq. (3.17d), $\alpha_{12} = \varsigma_{ii}$ is odd. Then $\varpi_{12} = (-1)^{\alpha_1+\alpha_2+\alpha_{12}+1} = (-1)^{2\varsigma_i+\varsigma_{ii}+1} = 1$ since $(-1)^{2\varsigma_i} = (-1)^{1+2\lambda_i} = 1$ (see Eq. (3.1)): $(-1)^{2\lambda_i} = (-1)^{1+2l_i} = -1$ ($l_i = 0, 1, \ldots$) for LS-coupling and $(-1)^{2\lambda_i} = (-1)^{2j_i} = -1$ ($j_i = 1/2, 3/2, \ldots$) for jj-coupling.

Consider two operators: $\widehat{\pi}_{132}\widehat{\mathcal{O}}^{\varsigma}_{\iota}([21]2)$, $\widehat{\pi}_{13}\widehat{\mathcal{O}}^{\varsigma}_{\iota}([21]2)$. The permutation representation $\widehat{\pi}_{132}$ is realised by the permutation $(132) = \left(\begin{smallmatrix}1&2&3\\3&1&2\end{smallmatrix}\right)$; the permutation representation $\widehat{\pi}_{13}$ acts on irreps α_s, $s = 1, 2, 3$ by transposing them with $(13) = \left(\begin{smallmatrix}1&2&3\\3&2&1\end{smallmatrix}\right)$. Consequently, the anticommutation rule in Eq. (3.2) enables us to write

$$\begin{aligned}\widehat{\pi}_{132}[W^{\varsigma_{ii}}(\lambda_i\lambda_i) \times a^{\varsigma_j}]^{\varsigma}_{\iota} &= [W^{\varsigma_{ij}}(\lambda_j\lambda_i) \times a^{\varsigma_i}]^{\varsigma}_{\iota} \equiv [W^{\alpha_{13}}(\lambda_3\lambda_1) \times a^{\alpha_2}]^{\alpha}_{\beta} \\ = \sum_{\varsigma_{ii}=\text{odd}} C_{132}[W^{\varsigma_{ii}}(\lambda_i\lambda_i) \times a^{\varsigma_j}]^{\varsigma}_{\iota} &\equiv \sum_{\alpha_{12}=\text{odd}} C_{132}[W^{\alpha_{12}}(\lambda_1\lambda_2) \times a^{\alpha_3}]^{\alpha}_{\beta},\end{aligned} \tag{3.46a}$$

$$C_{132} \overset{\text{def}}{=} \sum_{\substack{\iota_{i1}\iota_{i2}\\ \iota_j\iota_{ij}\iota_{ii}}} \langle\varsigma_j\iota_j\varsigma_i\iota_{i1}|\varsigma_{ij}\iota_{ij}\rangle\langle\varsigma_{ij}\iota_{ij}\varsigma_i\iota_{i2}|\varsigma\iota\rangle\langle\varsigma_i\iota_{i1}\varsigma_i\iota_{i2}|\varsigma_{ii}\iota_{ii}\rangle\langle\varsigma_{ii}\iota_{ii}\varsigma_j\iota_j|\varsigma\iota\rangle. \tag{3.46b}$$

The summation over indices causes the appearance of $6j$–symbols. However, it is unimportant in the present case. The transposition (13) permutes operators with the same value ς_i. Thus

$$\widehat{\pi}_{13}[W^{\varsigma_{ii}}(\lambda_i\lambda_i)\times a^{\varsigma_j}]^{\varsigma}_{\iota} = [W^{\varsigma_{ij}}(\lambda_j\lambda_i)\times a^{\varsigma_i}]^{\varsigma}_{\iota} \equiv [W^{\alpha_{23}}(\lambda_3\lambda_2)\times a^{\alpha_1}]^{\alpha}_{\beta}$$
$$= \sum_{\varsigma_{ii}=\text{odd}} C_{13}[W^{\varsigma_{ii}}(\lambda_i\lambda_i)\times a^{\varsigma_j}]^{\varsigma}_{\iota} + \delta(\varsigma_j,\varsigma)(-1)^{\varsigma_i+\varsigma_{ij}-\varsigma+1}[\varsigma_{ij}]^{1/2}[\varsigma]^{-1/2}a^{\varsigma}_{\iota}$$
$$\equiv \sum_{\alpha_{12}=\text{odd}} C_{13}[W^{\alpha_{12}}(\lambda_1\lambda_2)\times a^{\alpha_3}]^{\alpha}_{\beta} + \delta(\alpha_3,\alpha)(-1)^{\alpha_1+\alpha_{13}-\alpha+1}[\alpha_{13}]^{1/2}[\alpha]^{-1/2}a^{\alpha}_{\beta}, \tag{3.47a}$$

$$C_{13} \overset{\text{def}}{=} -\sum_{\substack{\iota_{i1}\iota_{i2}\\ \iota_j\iota_{ij}\iota_{ii}}} \langle\varsigma_j\iota_j\varsigma_i\iota_{i2}|\varsigma_{ij}\iota_{ij}\rangle\langle\varsigma_{ij}\iota_{ij}\varsigma_i\iota_{i1}|\varsigma\iota\rangle\langle\varsigma_i\iota_{i1}\varsigma_i\iota_{i2}|\varsigma_{ii}\iota_{ii}\rangle\langle\varsigma_{ii}\iota_{ii}\varsigma_j\iota_j|\varsigma\iota\rangle. \tag{3.47b}$$

In Eq. (3.47b), the third CGC equals to $\langle\varsigma_i\iota_{i1}\varsigma_i\iota_{i2}|\varsigma_{ii}\iota_{ii}\rangle = -\varpi_{12}\langle\varsigma_i\iota_{i2}\varsigma_i\iota_{i1}|\varsigma_{ii}\iota_{ii}\rangle$. But $\varpi_{12}=1$. Replace $\varsigma_i\iota_{i1}$ with $\varsigma_i\iota_{i2}$ in Eq. (3.46b). Then

$$C_{132} = C_{13}. \tag{3.48}$$

Eq. (3.48) has a significant meaning that makes sense for any operator $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$. A generalisation is straightforward due to the structure of coefficients C_{13}, C_{132}: it is a product of CGCs. Consequently, it is a manner of quantity of transpositions that permute the same value irreps only, but for both even and odd permutations, the coefficients coincide with each other because for any equal irreps α_s, $\alpha_{s'}$, the phase multiplier $\varpi_{ss'}=1$. Thus for the map $\tau_{\xi}\circ p_{13}\circ p_{23}\circ\tau^{-1}_{\xi'}$, $\mathcal{E}^{132}_{\xi'\xi} = \mathcal{E}^{13}_{\xi'\xi}$. Indeed, $(132)=(13)(23)$ and

$$\widehat{\pi}_{132}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12) = \widehat{\pi}_{13}\sum_{\alpha_{12}}\varepsilon_{23}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12) = \sum_{\alpha_{12}}\varepsilon_{(13)(23)}\varepsilon_{13}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12)$$
$$= \sum_{\alpha_{12}}\varepsilon_{132}\widehat{\mathcal{O}}^{\alpha}_{\beta}([2^21^2]12),$$

where $\varepsilon_{(13)(23)} \equiv \widehat{\pi}_{13}\varepsilon_{23}$, $\xi=\xi'=14$. Write $\varepsilon_{132} = \varepsilon_{13}\varepsilon_{(13)(23)}$. But $\varepsilon_{23} = \sum_{\alpha_{23}}\varpi_{23}\epsilon_6\epsilon_{(23)(6)}$ (see Eq. (3.34)). Thus $\varepsilon_{(13)(23)} = \sum_{\alpha_{12}}\epsilon_{(13)(6)}\epsilon_{(132)(6)}$, as $\widehat{\pi}_{13}\varpi_{23} = \varpi_{12} = 1$. Now refer to Eq. (A.6a) in Appendix A. This implies $\epsilon_{(13)(6)} = \epsilon_{(132)(6)} = \epsilon_6$. Then $\varepsilon_{(13)(23)} = \sum_{\alpha_{12}}\epsilon_6^2 = 1$ (see Eq. (3.13)), recalling that $\alpha_1=\alpha_2$ and thus $\alpha_{13}=\alpha_{23}$. The result is $\varepsilon_{132}=\varepsilon_{13}$.

The map $\tau_{\xi}\circ p_{13}\circ p_{23}\circ\tau^{-1}_{\xi'}\colon\ \mathscr{T}^{[\lambda']}_{\varkappa'} \longrightarrow (\widehat{\pi}_{132}\mathscr{T})^{[\lambda]}_{\varkappa}$ is realised through the coefficient (see Eq. (3.24))

$$\mathcal{E}^{132}_{\xi'\xi} = \sum_{\alpha_{\eta\in\mathcal{N}_{\xi'\xi}}}\varepsilon_{132}\epsilon_{\xi'}\epsilon_{(132)(\xi)}.$$

It has been already pointed out that $\varepsilon_{132}=\varepsilon_{13}$. The coefficient $\epsilon_{(132)(\xi)} = \epsilon_{(13)(\xi)}$: for $\widehat{\pi}_{13}$, $\alpha_1\leftrightarrow\alpha_3$; for $\widehat{\pi}_{132}$, $\alpha_1\to\alpha_3$, $\alpha_2\to\alpha_1$, $\alpha_3\to\alpha_2$, therefore $(\alpha_1=\alpha_2)$ $\alpha_1\to\alpha_3$, $\alpha_3\to\alpha_1 \Rightarrow$ $\alpha_1\leftrightarrow\alpha_3$. Then

$$\mathcal{E}^{132}_{\xi'\xi} = \sum_{\alpha_{\eta\in\mathcal{N}_{\xi'\xi}}}\varepsilon_{13}\epsilon_{\xi'}\epsilon_{(13)(\xi)} = \mathcal{E}^{13}_{\xi'\xi}.$$

It turns out that although a one-to-one correspondence $\tau_{\xi}\circ p_{13}\circ\tau^{-1}_{\xi'}\colon\ \mathscr{T}^{[\lambda']}_{\varkappa'} \longrightarrow (\widehat{\pi}_{13}\mathscr{T})^{[\lambda]}_{\varkappa}$ does not exist (the permutation of equal representations causes additional terms due to non-zero Kronecker deltas), but the realisation of a bijective map $\tau_{\xi}\circ p_{13}\circ p_{23}\circ\tau^{-1}_{\xi'}\colon\ \mathscr{T}^{[\lambda']}_{\varkappa'} \longrightarrow (\widehat{\pi}_{132}\mathscr{T})^{[\lambda]}_{\varkappa}$ is actualised by the coefficient $\mathcal{E}^{13}_{\xi'\xi}$ that relates operators $\widehat{\pi}_{13}\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ and $\widehat{\mathcal{O}}^{\alpha}([\lambda']\varkappa')$ if only $\alpha_1\neq\alpha_2$, that is, if only the map $\tau_{\xi}\circ p_{13}\circ\tau^{-1}_{\xi'}$ is valid.

A generalisation is plain due to the peculiarity of method based on commutative diagrams (Sec. 3.1.3). That is, each permutation operator $\widehat{\pi}$ realises a permutation π of irreps $\alpha_1,\alpha_2,\ldots$ by making the transformations so that only the irreps α_s and $\alpha_{s'}$ within $W^{\alpha_{ss'}}(\lambda_s\lambda_{s'})$ are permuted (the maps τ_{ξ}, τ^{-1}_{ξ}). If the irreducible tensor operator $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ associated to the scheme $\mathscr{T}^{[\lambda]}_{\varkappa}$ contains a set of several irreps α_s that are equal, then a minimal cardinality of such set is

2. Assume that a set K_t contains $2 \leq t < \ell$ equal irreps α_s. A particular condition $t = \ell$ is excessive because the permutations for the operators $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ with all equal irreps make no sense. Then it is always possible to find such two irreps $\alpha_s, \alpha_{s'} \in K_t$ that making transformations a given scheme $\mathscr{T}_{\varkappa}^{[\lambda]}$ is mapped to $\mathscr{T}_{\varkappa'}^{[\lambda']}$ which contains both $\alpha_s, \alpha_{s'} \in K_t$ that are now adjacent to one another. But this is a case of studied above operator $\widehat{\mathcal{O}}^{\alpha}([21]2)$ with $\alpha_1 = \alpha_2$. Consequently, all the rest operations are to be performed in the same manner.

3.2 Special cases

The section studies irreducible tensor operators $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ associated to some special angular reduction schemes $\mathscr{T}_{\varkappa}^{[\lambda]}$ that are particular in applications of theoretical atomic physics.

Two irreducible tensor spaces are considered (see Sec. 2.3): $\mathcal{H}^{\lambda}$ and $\mathcal{H}^{q}$. In Sec. 3.1.2, it was demonstrated that the irreducible tensor operators $\widehat{\mathcal{O}}^{\lambda}([1^2]1)$ or $\widehat{\mathcal{O}}^{\alpha}([1^2]1)$ associated to the angular reduction scheme $\mathscr{T}_1^{[1^2]}$ are—apart from a^{λ} ($\tilde{a}^{\lambda}$) or a^{α}—the building blocks of other irreducible tensor operators. The correspondence of a^{λ}, $\tilde{a}^{\lambda}$, $\widehat{\mathcal{O}}^{\lambda}([1^2]1)$ and a^{α}, $\widehat{\mathcal{O}}^{\alpha}([1^2]1)$ is displayed in Tab. 6, where a usual notation $\widehat{\mathcal{O}}^{\lambda}([1^2]1) \equiv W^{\lambda}$ ($\widehat{\mathcal{O}}^{\alpha}([1^2]1) \equiv W^{\alpha}$) is selected recalling that $\alpha \equiv \kappa\lambda$. A particular irreducible tensor operator $W^{\lambda}(\lambda_i\widetilde{\lambda}_j)$ ($W^{\alpha}(\lambda_i\lambda_j)$) represents a reduced $\widehat{O}_1$.

For the operator string $\widehat{O}_2$, two typical angular reduction schemes are observed in atomic physics, one that is traced to $\mathscr{T}_1^{[2^2]}$, and the other to $(\widehat{\pi}_{243}\mathscr{T})_1^{[2^2]}$. Following by Refs. [54,77,81], these schemes are accordingly called z-scheme and b-scheme. The associated irreducible tensor operators $\widehat{\mathcal{O}}^{\lambda}([2^2]1)$ and $\widehat{\pi}_{243}\widehat{\mathcal{O}}^{\lambda}([2^2]1)$ are related by

Tab. 6: A connection between irreducible tensor operators on $\mathcal{H}^{\lambda}$ and $\mathcal{H}^{q}$

$\widehat{\mathcal{O}}^{\lambda}_{\mu}$	$\widehat{\mathcal{O}}^{\alpha}_{\beta}$	$\widehat{\mathcal{O}}^{\lambda}_{\mu}$	$\widehat{\mathcal{O}}^{\alpha}_{\beta}$
a^{λ}_{μ}	$a^{\frac{1}{2}\,\lambda}_{\frac{1}{2}\,\mu}$	$W^{\lambda}_{\mu}(\lambda_i\widetilde{\lambda}_j)$	$\frac{1}{\sqrt{2}}\big(W^{0\lambda}_{0\mu}(\lambda_i\lambda_j) + W^{1\lambda}_{0\mu}(\lambda_i\lambda_j)\big)$
$\tilde{a}^{\lambda}_{\mu}$	$a^{\frac{1}{2}\,\lambda}_{-\frac{1}{2}\,\mu}$	$W^{\lambda}_{\mu}(\widetilde{\lambda}_i\lambda_j)$	$\frac{1}{\sqrt{2}}\big(-W^{0\lambda}_{0\mu}(\lambda_i\lambda_j) + W^{1\lambda}_{0\mu}(\lambda_i\lambda_j)\big)$
$W^{\lambda}_{\mu}(\lambda_i\lambda_j)$	$W^{1\lambda}_{1\mu}(\lambda_i\lambda_j)$	$W^{\lambda}_{\mu}(\lambda_i\widetilde{\lambda}_i)$	$\frac{1}{\sqrt{2}}W^{1\lambda}_{0\mu}(\lambda_i\lambda_i)$
$W^{\lambda}_{\mu}(\widetilde{\lambda}_i\widetilde{\lambda}_j)$	$W^{1\lambda}_{-1\mu}(\lambda_i\lambda_j)$	$W^{\lambda}_{\mu}(\widetilde{\lambda}_i\lambda_i)$	$\frac{1}{\sqrt{2}}W^{1\lambda}_{0\mu}(\lambda_i\lambda_i)$

$$\widehat{\pi}_{243}\widehat{\mathcal{O}}^{\lambda}([2^2]1) = [\lambda_{14},\lambda_{23}]^{1/2}\sum_{\lambda_{12}\lambda_{34}}\widehat{\mathcal{O}}^{\lambda}([2^2]1)(-1)^{\lambda_3+\lambda_4-\lambda_{34}}[\lambda_{12},\lambda_{34}]^{1/2}\begin{Bmatrix}\lambda_1 & \lambda_2 & \lambda_{12}\\ \lambda_4 & \lambda_3 & \lambda_{34}\\ \lambda_{14} & \lambda_{23} & \lambda\end{Bmatrix}$$
$$+\,\delta(\lambda_2,\lambda_4)\widehat{\mathcal{O}}^{\lambda}([1^2]1)(-1)^{\lambda_1-\lambda_2+\lambda_3+\lambda}[\lambda_{14},\lambda_{23}]^{1/2}\begin{Bmatrix}\lambda_1 & \lambda_3 & \lambda\\ \lambda_{23} & \lambda_{14} & \lambda_2\end{Bmatrix}. \quad (3.49)$$

Analogous relationship holds for the irreducible tensor operators $\widehat{\mathcal{O}}^{\alpha}([2^2]1)$ and $\widehat{\pi}_{243}\widehat{\mathcal{O}}^{\alpha}([2^2]1)$. A correspondence between $\widehat{\mathcal{O}}^{\lambda}([2^2]1)$ and $\widehat{\mathcal{O}}^{\alpha}([2^2]1)$ is actualised by the following linear combination

$$\tfrac{1}{\sqrt{3}}\widehat{\mathcal{O}}^{0\lambda}([2^2]1) + \tfrac{1}{\sqrt{2}}\widehat{\mathcal{O}}^{1\lambda}([2^2]1) + \tfrac{1}{\sqrt{6}}\widehat{\mathcal{O}}^{2\lambda}([2^2]1). \quad (3.50)$$

To compare with, a correspondence between $\widehat{\mathcal{O}}^{\lambda}([2^21^2]12)$ and $\widehat{\mathcal{O}}^{\alpha}([2^21^2]12)$ is actualised by

$$\tfrac{1}{2}\big(\widehat{\mathcal{O}}^{0\lambda}([2^21^2]12) + \widehat{\mathcal{O}}^{2\lambda}([2^21^2]12) + \tfrac{1}{\sqrt{5}}\{3\widehat{\mathcal{O}}^{1\lambda}([2^21^2]12) + \widehat{\mathcal{O}}^{3\lambda}([2^21^2]12)\}\big), \quad (3.51)$$

where $\mathscr{T}_{12}^{[2^21^2]}$ denotes the angular reduction scheme of $\widehat{O}_3$ (see Sec. 3.1).

3.2.1 Remark. Despite of different representations in distinct tensor spaces, it is by no means obvious that there exists a one-to-one correspondence of basis associated to irreducible tensor operators so that the matrix representations of $\widehat{\mathcal{O}}^{\lambda}$ and $\widehat{\mathcal{O}}^{\alpha}$ coincide. Consequently, the choice of considered tensor space is arbitrary and it depends on a specified subject matter.

3.2.1 A two-particle operator

In this section, the tensor properties of a two-particle operator—either physical or effective—are studied. The systematic study is essentially required due to the subsequent computation requirements needed to produce high-precision atomic structure data by generating large sets of matrix elements for a two-particle operator. The operator is of the form (refer to Eq. (2.69b))

$$\widehat{G}[\omega] \stackrel{\text{def}}{=} X_{\omega} \sum_{I_2} a_{\alpha} a_{\beta} a^{\dagger}_{\bar{\nu}} a^{\dagger}_{\bar{\mu}} \omega_{\alpha\beta\bar{\mu}\bar{\nu}}. \tag{3.52}$$

Much the same as in Sec. 2.3, the Greek letters $\alpha, \beta, \ldots$ designate the single-electron states characterised by the sets of numbers $\{n_{\alpha}, \lambda_{\alpha}, m_{\alpha}\}, \{n_{\beta}, \lambda_{\beta}, m_{\beta}\}, \ldots$. As usually, I_2 denotes the set of single-electron states. The multiplier X_{ω} is closely related to the structure of a two-particle matrix element $\omega_{\alpha\beta\bar{\mu}\bar{\nu}}$. If $\omega \equiv g$, that is, if $\widehat{G}[g] \equiv \widehat{G}$ denotes a two-particle operator representing some physical (Coulomb, Breit) interaction, then $X_{\omega} = 1/2$ and

$$g_{\alpha\beta\bar{\mu}\bar{\nu}} \stackrel{\text{def}}{=} \langle \alpha\beta | g_{12} | \bar{\mu}\bar{\nu} \rangle. \tag{3.53}$$

A two-particle matrix representation $g_{\alpha\beta\bar{\mu}\bar{\nu}}$ is sometimes useful to represent by [70, Eq. (38)]

$$g_{\alpha\beta\bar{\mu}\bar{\nu}} = 1/2\, \widetilde{g}_{\alpha\beta\bar{\mu}\bar{\nu}}, \quad \widetilde{g}_{\alpha\beta\bar{\mu}\bar{\nu}} \stackrel{\text{def}}{=} g_{\alpha\beta\bar{\mu}\bar{\nu}} - g_{\alpha\beta\bar{\nu}\bar{\mu}}. \tag{3.54}$$

Then for $\widehat{G}[\widetilde{g}] \equiv \widehat{G}^{A}$, $X_{\omega} = 1/4$. The superscript A over $\widehat{G}$ indicates the presence of antisymmetric two-particle matrix representation $\widetilde{g}_{\alpha\beta\bar{\mu}\bar{\nu}}$. For the symmetric and self-adjoint interaction operator $g_{12} = g_{21} = g^{\dagger}_{12}$, the symmetry properties of its matrix representations are

$$g_{\alpha\beta\bar{\mu}\bar{\nu}} = g_{\beta\alpha\bar{\nu}\bar{\mu}} = g_{\bar{\nu}\bar{\mu}\beta\alpha} = g_{\bar{\mu}\bar{\nu}\alpha\beta}, \tag{3.55a}$$

$$\begin{aligned} \widetilde{g}_{\alpha\beta\bar{\mu}\bar{\nu}} &= \widetilde{g}_{\beta\alpha\bar{\nu}\bar{\mu}} = \widetilde{g}_{\bar{\mu}\bar{\nu}\alpha\beta} = \widetilde{g}_{\bar{\nu}\bar{\mu}\beta\alpha} \\ &= -\widetilde{g}_{\alpha\beta\bar{\nu}\bar{\mu}} = -\widetilde{g}_{\beta\alpha\bar{\mu}\bar{\nu}} = -\widetilde{g}_{\bar{\mu}\bar{\nu}\beta\alpha} = -\widetilde{g}_{\bar{\nu}\bar{\mu}\alpha\beta}. \end{aligned} \tag{3.55b}$$

To find the irreducible tensor form of $\widehat{G}[\omega]$, a usual decomposition (see, for example, Eq. (3.5)) is performed.

$$\widehat{G}[\omega] = \sum_{I_2} \sum_{\Lambda} \sum_{M=-\Lambda}^{+\Lambda} \widehat{G}^{\Lambda}_{M}. \tag{3.56}$$

Each irreducible tensor operator $\widehat{G}^{\Lambda}$ acts on $\mathcal{H}^{\Lambda}$.

3.2.2 Remark. In the present section, operators acting on the irreducible tensor space $\mathcal{H}^{\Lambda}$ will be considered. Their correspondence to operators on $\mathcal{H}^{q}$ is associated by using the data in Tab. 6 and by applying Eq. (3.50).

For the irreducible tensor operators $\widehat{G}^{\Lambda}$ associated to the angular reduction scheme $\mathscr{T}_1^{[2^2]}$ (z-scheme), it is easy to deduce that

$$\widehat{G}^{\Lambda} \stackrel{\text{def}}{=} -\sum_{\Lambda_1\Lambda_2} [W^{\Lambda_1}(\lambda_{\alpha}\lambda_{\beta}) \times W^{\Lambda_2}(\widetilde{\lambda}_{\bar{\mu}}\widetilde{\lambda}_{\bar{\nu}})]^{\Lambda}\, \Omega_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda), \tag{3.57}$$

$$\Omega_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda) \stackrel{\text{def}}{=} \sum_{\substack{m_{\alpha}m_{\beta} \\ m_{\bar{\mu}}m_{\bar{\nu}}}} (-1)^{\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+m_{\bar{\mu}}+m_{\bar{\nu}}} E\begin{pmatrix} \lambda_{\alpha} & \lambda_{\beta} & \lambda_{\bar{\mu}} & \lambda_{\bar{\nu}} \\ m_{\alpha} & m_{\beta} & -m_{\bar{\mu}} & -m_{\bar{\nu}} \end{pmatrix}; \Lambda_1\Lambda_2\Lambda M \omega_{\alpha\beta\bar{\mu}\bar{\nu}}. \tag{3.58}$$

A decomposition in Eq. (3.56) is convenient to find matrix elements of $\widehat{G}[\omega]$ on the basis $|\Gamma_i \Pi_i \Lambda_i M_i\rangle$ which is a linear combination of CSFs (see Eq. (2.2)). That is, a matrix representation of $\widehat{G}[\omega]$ on exact wave functions is the sum of matrix representations of $\widehat{G}^{\Lambda}$ on the

eigenfunctions of atomic central-field Hamiltonian. Meanwhile, to find the matrix element of $\widehat{G}^{\Lambda}$ means to find the matrix element of $\widehat{\mathcal{O}}^{\Lambda}([2^2]1)$ given on the right hand side of Eq. (3.57). These particular matrix representations of $\widehat{\mathcal{O}}^{\Lambda}([2^2]1)$ have been comprehensively studied in Refs. [46, 50]. Consequently, to accomplish the formation of $\widehat{G}^{\Lambda}$, the basis-independent quantities $\Omega_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda)$ are to be found. These quantities are related to the origin of interaction operator (not necessarily physical) g_{12}, as demonstrated in Eq. (3.58), where, in general,

$$E\begin{pmatrix}\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4\\ \mu_1 & \mu_2 & \mu_3 & \mu_4\end{pmatrix}; \lambda_{12}\lambda_{34}\lambda\mu\Big) \stackrel{\text{def}}{=} \langle\lambda_1\mu_1\lambda_2\mu_2|\lambda_{12}\mu_{12}\rangle\langle\lambda_3\mu_3\lambda_4\mu_4|\lambda_{34}\mu_{34}\rangle \times \langle\lambda_{12}\mu_{12}\lambda_{34}\mu_{34}|\lambda\mu\rangle. \tag{3.59}$$

For some permutation representations $\widehat{\pi}$ of S_4, the coefficient E satisfies

$$\widehat{\pi}E\begin{pmatrix}\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4\\ \mu_1 & \mu_2 & \mu_3 & \mu_4\end{pmatrix}; \lambda_{12}\lambda_{34}\lambda\mu\Big) = \mathcal{Z}_{\pi(1)\pi(2)\pi(3)\pi(4)}(\lambda_{12}\lambda_{34}\lambda)E\begin{pmatrix}\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4\\ \mu_1 & \mu_2 & \mu_3 & \mu_4\end{pmatrix}; \lambda_{12}\lambda_{34}\lambda\mu_{\pi}\Big). \tag{3.60}$$

If $\pi = 1_4, (14)(23)$, then $\mathcal{Z}_{1234} = \mathcal{Z}_{4321} = 1$, $\mu_{1_4} = \mu$, $\mu_{(14)(23)} = -\mu$. If $\pi = (12), (1423)$, then $\mathcal{Z}_{2134} = \mathcal{Z}_{4312} = a(\lambda_1\lambda_2\lambda_{12})$, $\mu_{(12)} = \mu$, $\mu_{(1423)} = -\mu$ and $a(\lambda_1\lambda_2\lambda_{12}) \stackrel{\text{def}}{=} (-1)^{\lambda_1+\lambda_2+\lambda_{12}}$. If $\pi = (34), (1324)$, then $\mathcal{Z}_{1243} = \mathcal{Z}_{3421} = a(\lambda_3\lambda_4\lambda_{34})$, $\mu_{(34)} = \mu$ and $\mu_{(1324)} = -\mu$. Finally, if $\pi = (12)(34), (13)(24)$, then $\mathcal{Z}_{2143} = \mathcal{Z}_{3412} = a(\lambda_1\lambda_2\lambda_{12})a(\lambda_3\lambda_4\lambda_{34})$, $\mu_{(12)(34)} = \mu$ and $\mu_{(13)(24)} = -\mu$.

For the physical interactions g_{12}, the quantity $\Omega_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda)$ equals—up to a multiplier—to the reduced matrix element of g^{Λ}, where g^{Λ} is defined much the same as $\widehat{G}^{\Lambda}$ for $\widehat{G}[\omega]$ (see Eq. (3.56)). Indeed, if $g_{\alpha\beta\bar{\mu}\bar{\nu}}$ is calculated on the basis of single-electron eigenstates $|\alpha\rangle, \ldots, |\bar{\nu}\rangle$, then

$$\Omega_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda) = a(\lambda_{\bar{\mu}}, \lambda_{\bar{\nu}}, \Lambda_2)z(\Lambda\lambda_{\alpha}\lambda_{\beta}\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1\Lambda_2), \tag{3.61}$$

where

$$z(\Lambda\lambda_{\alpha}\lambda_{\beta}\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1\Lambda_2) \stackrel{\text{def}}{=} 1/2\ [\Lambda_1]^{1/2}[\Lambda]^{-1/2}[n_{\alpha}\lambda_{\alpha}n_{\beta}\lambda_{\beta}\Lambda_1\|g^{\Lambda}\|n_{\bar{\mu}}\lambda_{\bar{\mu}}n_{\bar{\nu}}\lambda_{\bar{\nu}}\Lambda_2] \tag{3.62}$$

or on the contrary

$$g_{\alpha\beta\bar{\mu}\bar{\nu}} = 2\sum_{\Lambda_1\Lambda_2\Lambda}(-1)^{\Lambda_2+m_{\bar{\mu}}+m_{\bar{\nu}}}\begin{pmatrix}\lambda_{\alpha} & \lambda_{\beta} & \lambda_{\bar{\mu}} & \lambda_{\bar{\nu}}\\ m_{\alpha} & m_{\beta} & -m_{\bar{\mu}} & -m_{\bar{\nu}}\end{pmatrix}; \Lambda_1\Lambda_2\Lambda M\Big)z(\Lambda\lambda_{\alpha}\lambda_{\beta}\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1\Lambda_2). \tag{3.63}$$

The coefficient z that represents the basis-independent part of $\widetilde{g}_{\alpha\beta\bar{\mu}\bar{\nu}}$ equals to

$$\widetilde{z}(\Lambda\lambda_{\alpha}\lambda_{\beta}\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1\Lambda_2) \stackrel{\text{def}}{=} z(\Lambda\lambda_{\alpha}\lambda_{\beta}\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1\Lambda_2) - a(\lambda_{\bar{\mu}}\lambda_{\bar{\nu}}\Lambda_2)z(\Lambda\lambda_{\alpha}\lambda_{\beta}\lambda_{\bar{\mu}}\lambda_{\bar{\nu}}\Lambda_1\Lambda_2). \tag{3.64}$$

Explicit expressions of z depend on a specified interaction operator g_{12}.

Example (*Coulomb interaction).* Assume that a single-electron eigenstate $|\alpha\rangle$ is a 4–spinor such that [82, p. 106, Eq. (19.2)]

$$|\alpha\rangle \equiv |n_{\alpha}l_{\alpha}j_{\alpha}m_{\alpha}\rangle = \begin{pmatrix} f(n_{\alpha}l_{\alpha}j_{\alpha}|r)|l_{\alpha}j_{\alpha}m_{\alpha}\rangle \\ (-1)^{\vartheta_{\alpha}}g(n_{\alpha}l'_{\alpha}j_{\alpha}|r)|l'_{\alpha}j_{\alpha}m_{\alpha}\rangle\end{pmatrix} \tag{3.65}$$

and $\vartheta_{\alpha} \stackrel{\text{def}}{=} l_{\alpha} - j_{\alpha} + 1/2$, $l'_{\alpha} \stackrel{\text{def}}{=} 2j_{\alpha} - l_{\alpha}$, $l_{\alpha} = j_{\alpha} \pm 1/2$. The 2–spinors $|l_{\alpha}j_{\alpha}m_{\alpha}\rangle$ are constructed as follows [52, Sec. 2.3, p. 13, Eq. (2.16)]

$$|l_{\alpha}j_{\alpha}m_{\alpha}\rangle \stackrel{\text{def}}{=} \sum_{\mu=-1/2}^{+1/2}\langle l_{\alpha}m_{\alpha}-\mu\ 1/2\ \mu|j_{\alpha}m_{\alpha}\rangle Y^{l_{\alpha}}_{m_{\alpha}-\mu}(\widehat{x})\begin{pmatrix}\delta(\mu,+1/2)\\ \delta(\mu,-1/2)\end{pmatrix}. \tag{3.66}$$

Then the matrix representation z of $1/r_{12}$ on the basis in Eq. (3.65) equals to

$$z(0l_{\alpha}j_{\alpha}l_{\beta}j_{\beta}l_{\bar{\nu}}j_{\bar{\nu}}l_{\bar{\mu}}j_{\bar{\mu}}J_1J_2) = 1/2\ \delta(J_1,J_2)(-1)^{j_{\alpha}-j_{\bar{\nu}}+(l_{\bar{\mu}}+l_{\bar{\nu}}-l_{\alpha}-l_{\beta})/2}$$
$$\times\ [j_{\alpha},j_{\beta},j_{\bar{\mu}},j_{\bar{\nu}},J_1]^{1/2}\sum_k[k]^{-1}\begin{Bmatrix}j_{\alpha} & j_{\bar{\mu}} & k\\ j_{\bar{\nu}} & j_{\beta} & J_1\end{Bmatrix}\langle j_{\alpha}1/2\ j_{\bar{\mu}}\ -1/2|k0\rangle\langle j_{\beta}1/2\ j_{\bar{\nu}}\ -1/2|k0\rangle$$

$$\times \big(R_k(\alpha\beta,\bar\mu\bar\nu)+R_k(\alpha\beta',\bar\mu\bar\nu')+R_k(\alpha'\beta,\bar\mu'\bar\nu)+R_k(\alpha'\beta',\bar\mu'\bar\nu')\big). \tag{3.67}$$

The radial integrals R_k are defined in Ref. [52, Sec. 19.3, p. 232, Eq. (19.72)]. The primes over single-electron states designate the corresponding small component g of relativistic radial wave function.

Example (*Coulomb interaction #2).* Bhatia et. al. [65, Sec. 5, Eq. (55)] constructed a total two-electron wave function so that for $S=0,1$,

$$|\Pi_{12}LSM\rangle = {\sum_\kappa}'' \big[f_\kappa^+({}^{2S+1}L|r_1,r_2)\mathcal{D}^{L\,+}_{M\kappa}(\Omega)+f_\kappa^-({}^{2S+1}L|r_1,r_2)\mathcal{D}^{L\,-}_{M\kappa}(\Omega)\big],\quad \Pi_{12}=(-1)^{l_1+l_2}.$$

The sum with double prime runs over $\kappa=0,2,\dots,k\le L$, $k\in 2\mathbb{Z}^+$ if parity $\Pi_{12}=1$ and over $\kappa=1,3,\dots,k\le L$, $k\in 2\mathbb{Z}^+ +1$ if parity $\Pi_{12}=-1$. The radial functions satisfy

$$\begin{aligned} f_\kappa^+({}^1L|r_2,r_1) &= (-1)^{L+\kappa}f_\kappa^+({}^1L|r_1,r_2), & f_\kappa^-({}^1L|r_2,r_1) &= (-1)^{L+\kappa+1}f_\kappa^-({}^1L|r_1,r_2),\\ f_\kappa^+({}^3L|r_2,r_1) &= (-1)^{L+\kappa+1}f_\kappa^+({}^3L|r_1,r_2), & f_\kappa^-({}^3L|r_2,r_1) &= (-1)^{L+\kappa}f_\kappa^-({}^3L|r_1,r_2). \end{aligned}$$

The radial equations for $f_\kappa^\pm$ are listed in Eq. (70) of Ref. [65], where it is also demonstrated that they are the same as that of Breit [83]. $\Omega\equiv(\Phi,\Theta,\Psi)$ denotes the usual Euler angles that connect the coordinates $\widehat{x}_1$, $\widehat{x}_2$ of both electrons. The spherical functions $\mathcal{D}^{L\,\pm}_{M\kappa}(\Omega)$ are defined by

$$\begin{aligned} \mathcal{D}^{L\,+}_{M\kappa}(\Omega) &\stackrel{\text{def}}{=} \frac{D^L_{M\kappa}(\Omega)+(-1)^\kappa D^L_{M-\kappa}(\Omega)}{\sqrt{2}\big[1+\delta(\kappa,0)(\sqrt{2}-1)\big]},\\ \mathcal{D}^{L\,-}_{M\kappa}(\Omega) &\stackrel{\text{def}}{=} \frac{D^L_{M\kappa}(\Omega)-(-1)^\kappa D^L_{M-\kappa}(\Omega)}{\sqrt{2}\,\mathrm{i}}. \end{aligned}$$

To find the matrix representation z of $1/r_{12}$, it is more convenient to introduce the radial function

$$\begin{aligned} g_\mu({}^{2S+1}L|r_1,r_2) &\stackrel{\text{def}}{=} {}^1\!/\!_{\sqrt{2}}\,\big[f_\mu^+({}^{2S+1}L|r_1,r_2)-\mathrm{i}f_\mu^-({}^{2S+1}L|r_1,r_2)\big], && \text{for } \mu\ge 0,\\ g_\mu({}^{2S+1}L|r_1,r_2) &\stackrel{\text{def}}{=} {}^{(-1)^\mu}\!/\!_{\sqrt{2}}\,\big[f_{|\mu|}^+({}^{2S+1}L|r_1,r_2)+\mathrm{i}f_{|\mu|}^-({}^{2S+1}L|r_1,r_2)\big], && \text{for } \mu<0 \end{aligned}$$

which leads to a compact form [65, Sec. 5, Eq. (47)]

$$|\Pi_{12}LSM\rangle = \sum_{\mu=-L}^{L} g_\mu({}^{2S+1}L|r_1,r_2)D^L_{M\mu}(\Omega). \tag{3.68}$$

Eq. (3.68) is convenient to apply the RCGC technique suggested in Sec. 2.2.2, whereas the spherical functions $D^L_{M\mu}(\Omega)$ are the eigenfunctions of Laplacian on $\mathrm{SU}(2)$ [62, Sec. III-4.8, p. 14, Eq. (5)]

$$\Delta_\Omega \stackrel{\text{def}}{=} \frac{\partial^2}{\partial\Theta^2}+\cot\Theta\,\frac{\partial}{\partial\Theta}+\frac{1}{\sin^2\Theta}\left(\frac{\partial^2}{\partial\Phi^2}-2\cot\Theta\,\frac{\partial^2}{\partial\Phi\partial\Psi}+\frac{\partial^2}{\partial\Psi^2}\right),$$

much the same as the spherical harmonics $Y^L_M(\widehat{x})$ are the eigenfunctions of Laplacian $\Delta_{\widehat{x}}$ [11, Sec. I-1, p. 13, Eq. (1.4)] on $\mathrm{SO}(3)$. By using Eq. (2.37), it is easy to deduce that

$$\begin{aligned} z(00l_\alpha l_\beta l_{\bar\nu}l_{\bar\mu}L_1S_1L_2S_2) &= 2\pi\delta(\Pi_{\alpha\beta},\Pi_{\bar\mu\bar\nu})\delta(L_1,L_2)\delta(S_1,S_2)[L_1]^{-1/2}\\ &\times\sum_{k\in 2\mathbb{Z}^+}(-1)^k[k]^{-1}[k\|\mathcal{S}^k\|k]\sum_{Q=-k}^{k}\langle k0kQ|kQ\rangle\sum_{\varkappa=-L_1}^{L_1}F^k_\varkappa({}^{2S_1+1}L_1), \end{aligned} \tag{3.69}$$

where the radial integral

$$F^k_\varkappa({}^{2S+1}L)\stackrel{\text{def}}{=}\iint_{\mathbb{R}^+}\mathrm{d}r_1\mathrm{d}r_2\;r_1^2r_2^2\,\frac{r_<^k}{r_>^{k+1}}\;\big|g_\varkappa({}^{2S+1}L|r_1,r_2)\big|^2.$$

Reduced matrix elements of the $\mathrm{SO}(3)$–irreducible tensor operators (Proposition 2.2.3) $\mathcal{S}^k$ are found from Eq. (2.38). For the detailed study of radial functions $g_\varkappa$, see Ref. [65, Sec. VII, p. 1057].

Example (*Magnetic interaction*). One of the components of Breit operator is the so-called magnetic interaction $[-(\alpha_1^1 \cdot \alpha_2^1)]/r_{12}$, where each Dirac matrix α_i^1 is referred to the ith electron. The irreducible tensor form of magnetic interaction can be found in Ref. [84, Sec. 2-5, p. 67, Eq. (5.86a)]. Then the matrix representation z on the 4–spinors (see Eq. (3.65)) obeys the form

$$z(0l_\alpha j_\alpha l_\beta j_\beta l_{\bar\nu} j_{\bar\nu} l_{\bar\mu} j_{\bar\mu} J_1 J_2) = {}^1\!/_2\,\delta(J_1,J_2)(-1)^{j_\alpha - j_{\bar\nu} + (l_{\bar\mu}+l_{\bar\nu}-l_\alpha-l_\beta)/2}[j_\alpha, j_\beta, j_{\bar\mu}, j_{\bar\nu}, J_1]^{1/2}$$
$$\times \sum_{kK}(-1)^{K+k}[k]^{-1}\begin{Bmatrix} j_\alpha & j_{\bar\mu} & K \\ j_{\bar\nu} & j_\beta & J_1 \end{Bmatrix}\langle j_\alpha {}^1\!/_2\; j_{\bar\mu}\; -{}^1\!/_2 | K0\rangle\langle j_\beta {}^1\!/_2\; j_{\bar\nu}\; -{}^1\!/_2 | K0\rangle$$
$$\times R_k(\alpha\beta\bar\nu\bar\mu)\mathcal{M}F_{kkK}(\alpha\beta\bar\nu\bar\mu), \tag{3.70}$$

$$R_k(\alpha\beta\bar\nu\bar\mu) \stackrel{\text{def}}{=} \big(R_k(\alpha'\beta',\bar\mu\bar\nu) \quad R_k(\alpha'\beta,\bar\mu\bar\nu') \quad R_k(\alpha\beta',\bar\mu'\bar\nu) \quad R_k(\alpha\beta,\bar\mu'\bar\nu')\big), \tag{3.71}$$

$$\mathcal{M} \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}, \quad F_{k_1k_2K}(\alpha\beta\bar\nu\bar\mu) \stackrel{\text{def}}{=} \begin{pmatrix} A(k_1,K)A(k_2,K) \\ A(k_1,K)B_{\beta\bar\nu}(k_2,K) \\ B_{\alpha\bar\mu}(k_1,K)A(k_2,K) \\ B_{\alpha\bar\mu}(k_1,K)B_{\beta\bar\nu}(k_2,K) \end{pmatrix}, \tag{3.72}$$

$$A(k,K) \stackrel{\text{def}}{=} {}^1\!/_2[1-(-1)^{K+k}]\langle 10K0|k0\rangle, \tag{3.73}$$

$$B_{\rho\sigma}(k,K) \stackrel{\text{def}}{=} (-1)^{K+k+l_\sigma+j_\sigma-\frac{1}{2}}\frac{[j_\sigma]+(-1)^{j_\rho+j_\sigma+K}[j_\rho]}{\sqrt{2K(K+1)}}\langle 11K\;-1|k0\rangle \tag{3.74}$$

with $\rho\sigma \equiv \alpha\bar\mu$ and $\rho\sigma \equiv \beta\bar\nu$.

Example (*Retarding interaction*). The second (and the last) component of relativistic Breit operator is the so-called interaction of retardation $[-(\alpha_1^1 \cdot \nabla_1^1)(\alpha_2^1 \cdot \nabla_2^1)]r_{12}/2$ whose irreducible tensor form is given in Ref. [84, Sec. 2-5, p. 67, Eq. (5.87a)]. The matrix representation

$$z(0l_\alpha j_\alpha l_\beta j_\beta l_{\bar\nu} j_{\bar\nu} l_{\bar\mu} j_{\bar\mu} J_1 J_2) = {}^1\!/_2\,\delta(J_1,J_2)(-1)^{j_\alpha - j_{\bar\nu} + (l_{\bar\mu}+l_{\bar\nu}-l_\alpha-l_\beta)/2}[j_\alpha, j_\beta, j_{\bar\mu}, j_{\bar\nu}, J_1]^{1/2}$$
$$\times \sum_k \Bigg([k]^{-1}\frac{k}{2k-1}\begin{Bmatrix} j_\alpha & j_{\bar\mu} & k-1 \\ j_{\bar\nu} & j_\beta & J_1 \end{Bmatrix}\langle j_\alpha {}^1\!/_2\; j_{\bar\mu}\; -{}^1\!/_2 | k-1\;0\rangle\langle j_\beta {}^1\!/_2\; j_{\bar\nu}\; -{}^1\!/_2 | k-1\;0\rangle$$
$$\times R_k(\alpha\beta\bar\nu\bar\mu)\mathcal{M}F_{kkk-1}(\alpha\beta\bar\nu\bar\mu) + \frac{\sqrt{k+1}}{2k+3}\begin{Bmatrix} j_\alpha & j_{\bar\mu} & k+1 \\ j_{\bar\nu} & j_\beta & J_1 \end{Bmatrix}\langle j_\alpha {}^1\!/_2\; j_{\bar\mu}\; -{}^1\!/_2 | k+1\;0\rangle$$
$$\times \langle j_\beta {}^1\!/_2\; j_{\bar\nu}\; -{}^1\!/_2 | k+1\;0\rangle \Big([k]^{-1}\sqrt{k+1}R_k(\alpha\beta\bar\nu\bar\mu)\mathcal{M}F_{kkk+1}(\alpha\beta\bar\nu\bar\mu) + \frac{\sqrt{k+2}}{2}$$
$$\times \big[P_k^{(12)}(\alpha\beta\bar\nu\bar\mu)\mathcal{M}F_{kk+2\,k+1}(\alpha\beta\bar\nu\bar\mu) + P_k^{(21)}(\alpha\beta\bar\nu\bar\mu)\mathcal{M}F_{k+2\,k\,k+1}(\alpha\beta\bar\nu\bar\mu)\big]\Big)\Bigg). \tag{3.75}$$

Matrices $R_k(\alpha\beta\bar\nu\bar\mu)$, $\mathcal{M}$ and $F_{k_1k_2K}$ are defined in Eqs. (3.71)-(3.72). The matrix $P_k^{(ij)}(\alpha\beta\bar\nu\bar\mu)$ is considered by

$$P_k^{(ij)}(\alpha\beta\bar\nu\bar\mu) \stackrel{\text{def}}{=} \big(P_k^{(ij)}(\alpha'\beta',\bar\mu\bar\nu) \quad P_k^{(ij)}(\alpha'\beta,\bar\mu\bar\nu') \quad P_k^{(ij)}(\alpha\beta',\bar\mu'\bar\nu) \quad P_k^{(ij)}(\alpha\beta,\bar\mu'\bar\nu')\big), \tag{3.76}$$

where the radial integral $P_k^{(ij)}(\alpha\beta,\bar\mu\bar\nu)$ is considered in the same way as $R_k(\alpha\beta,\bar\mu\bar\nu)$ by replacing $r_<^k/r_>^{k+1}$ with $r_i^{k+2}/r_j^{k+3} - r_i^k/r_j^{k+1}$.

3.2.3 Remark. From the above studied examples it appears that the physical two-particle operators $g^\Lambda = g^0$ observed in atomic physics are scalars. This significantly simplifies further on calculations. On the other hand, it is not necessary true for the effective two-particle operators.

The irreducible tensor operators $\widehat{G}^\Lambda$ associated to the angular reduction scheme $(\widehat{\pi}_{243}\mathscr{T})_1^{[2^2]}$ (b-scheme) are derived from the irreducible tensor operators $\widehat{G}^\Lambda$ associated to $\mathscr{T}_1^{[2^2]}$ by using Eq. (3.49) which clearly establishes the sum of two irreducible tensor operators. Consequently, the scheme $(\widehat{\pi}_{243}\mathscr{T})_1^{[2^2]}$ is less convenient from the point of view of tensor structure derived from Eq. (3.52). On the other hand, whilst on the subject of a particular operator, the present reduction scheme is more preferable to compare with $\mathscr{T}_1^{[2^2]}$, as it provides information related to the inner structure of g^Λ expressly. This is easily seen from the equation

$$g_{\alpha\beta\bar{\mu}\bar{\nu}} = 2 \sum_{\Lambda_1'\Lambda_2'\Lambda} (-1)^{\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+m_{\bar{\mu}}+m_{\bar{\nu}}} E\begin{pmatrix} \lambda_\alpha & \lambda_{\bar{\mu}} & \lambda_\beta & \lambda_{\bar{\nu}} \\ m_\alpha & -m_{\bar{\mu}} & m_\beta & -m_{\bar{\nu}} \end{pmatrix}; \Lambda_1'\Lambda_2'\Lambda M\Big) \times b(\Lambda\lambda_\alpha\lambda_\beta\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1'\Lambda_2'), \tag{3.77}$$

where b coefficient is such that

$$z(\Lambda\lambda_\alpha\lambda_\beta\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1\Lambda_2) = (-1)^{\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+\Lambda_2}[\Lambda_1,\Lambda_2]^{1/2} \sum_{\Lambda_1'\Lambda_2'} [\Lambda_1',\Lambda_2']^{1/2} \begin{Bmatrix} \lambda_{\bar{\mu}} & \lambda_{\bar{\nu}} & \Lambda_2 \\ \Lambda_1' & \Lambda_2' & \Lambda \\ \lambda_\alpha & \lambda_\beta & \Lambda_1 \end{Bmatrix} \times b(\Lambda\lambda_\alpha\lambda_\beta\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}\Lambda_1'\Lambda_2'). \tag{3.78}$$

In Eq. (3.77), the structure of E indicates that the irreps Λ_1', Λ_2'—despite of a resultant irrep Λ—designate intermediate irreps of g^Λ that is found by applying a usual technique of separation of variables (coordinates). That is,

$$g^\Lambda = \sum_{\Lambda_1'\Lambda_2'} g(r_1,r_2)[g^{\Lambda_1'}(\widehat{x}_1) \times g^{\Lambda_2'}(\widehat{x}_2)]^\Lambda, \tag{3.79}$$

where $g(r_1,r_2)$ is a radial function. Conversely, the coefficient E in Eq. (3.63) involves the irreps Λ_1, Λ_2 that are supplemental, as it is demonstrated in Eq. (3.78). For this reason, the angular reduction scheme $\mathscr{T}_1^{[2^2]}$ supplies more versatility to compare with $(\widehat{\pi}_{243}\mathscr{T})_1^{[2^2]}$, but at the same time it leads to additional summations. The latter fact, however, will be argued against when studying the two-particle effective matrix elements $\omega_{\alpha\beta\bar{\mu}\bar{\nu}}$ in more detail (Sec. 4).

Another circumstance of a widespread application of b-scheme is that for LS-coupling, the irreducible tensor operators $\widehat{\pi}_{243}\widehat{\mathcal{O}}^\lambda([2^2]1)$ are simply the tensor products of generators $W^{\lambda_{\alpha\bar{\mu}}}$, $W^{\lambda_{\beta\bar{\nu}}}$ of accordingly $\mathrm{U}(N_{l_\alpha})$, $\mathrm{U}(N_{l_\beta})$ if $l_\alpha = l_{\bar{\mu}}$ and $l_\beta = l_{\bar{\nu}}$ (recall that $N_l = 4l+2$). But this is a case of equivalent electrons of atom. The Lie algebra of the present generators is expressly defined and studied in Ref. [50, Sec. 6, p. 46, Eq. (6.20)]. The b coefficients in $\mathcal{H}^q$ space were first originated by Kaniauskas et. al. [85, Eq. (2.11)]. Later, the representation of operators in b-scheme found many applications in theoretical atomic spectroscopy [14,15,54,55,81,87] as well as in MBPT [36, 37, 86, 88]. In contrast, a more versatile z-scheme that was first systematically developed in Refs. [77, 81] found a natural application to the effective operator approach in MBPT [72, 73]. The present technique is considered in Sec. 4.

The efficiency of calculation of matrix elements—as a principal motive—strongly depends on the preparation of expressions of the irreducible tensor operators $\widehat{G}^\Lambda$. In atomic physics, a typical task is to calculate the matrix element of $\widehat{G}^\Lambda$ that acts on $\ell = 1,2,3,4$ electron shells of atom. Consequently, the values of irreps λ_α, λ_β, $\lambda_{\bar{\mu}}$, $\lambda_{\bar{\nu}}$ in $\widehat{\mathcal{O}}^\Lambda([2^2]1)$ depend on ℓ. Particularly, if $\ell = 1$, then $\lambda_\alpha = \lambda_\beta = \lambda_{\bar{\mu}} = \lambda_{\bar{\nu}}$; if $\ell = 4$, then $\lambda_\alpha \neq \lambda_\beta \neq \lambda_{\bar{\mu}} \neq \lambda_{\bar{\nu}}$. Possible preparations of $\widehat{G}^\Lambda$ that acts on $\ell = 1,2,3,4$ electron shells are displayed in Ref. [14, Tab. 1], where both schemes are mixed depending on a specified case, and in Ref. [77, Tabs. 1-3], where both schemes are strictly separated. It is to be noted the essential difference between methods used in these two works: it is a manner of distribution of irreps and of the choice of angular reduction scheme. The following example of application of b-scheme clearly demonstrates that. Assume that $\ell = 4$. In Ref. [77, Tab. 3, case:$\varrho = 1$], the irreducible tensor operator $\widehat{\mathcal{O}}^\Lambda([21^2]1)$ associated to the angular reduction scheme $\mathscr{T}_1^{[21^2]}$ (Tab. 3) is considered, while in Ref. [14, Fig. A1, A_7], the irreducible tensor operator $\widehat{\mathcal{O}}^\Lambda([2^2]1)$ associated to $\mathscr{T}_1^{[2^2]}$ is preferred. As a result, in the first approach, the angular coefficient contains a product of two $6j$–symbols; in the second approach [14, Eq. (52)], the angular coefficient contains a $9j$–symbol, though.

3.2.2 A three-particle operator

Unlike the case of a two-particle operator, the study of a three-particle operator is much more complicated and not so well fulfilled. First attempts to clarify the tensor structure of scalar three-particle operators belong to Judd [47, 89] who specified on the classification of terms of f^N configuration. Later, Leavitt et. al. [49, 90, 91] comprehensively considered effective three-particle operators acting within the d, f shells. Recently, a few works [42, 92, 93] devoted to the

effective operator approach that accounts for triple excitations are found. None of them provide a systematic classification of operators acting on $\ell = 2, 3, \ldots, 6$ electron shells.

A three-particle operator is of the form (refer to Eq. (2.69c))

$$\widehat{L} \stackrel{\text{def}}{=} \sum_{I_3} a_\alpha a_\beta a_\varsigma a^\dagger_{\bar\eta} a^\dagger_{\bar\nu} a^\dagger_{\bar\mu}\, \omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}. \tag{3.80}$$

The effective three-particle matrix element $\omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}$ depends on the case under consideration. However, formally the Wigner–Eckart theorem can be applied. The result reads

$$\widehat{L} = \sum_{I_3} \sum_{\Lambda} \sum_{M=-\Lambda}^{+\Lambda} \widehat{L}^\Lambda, \tag{3.81}$$

where the irreducible tensor operator $\widehat{L}^\Lambda$ acts on $\mathcal{H}^\Lambda$ and it is associated to the angular reduction scheme $\mathscr{T}_{12}^{[2^21^2]}$ (Tab. 4) so that

$$\begin{aligned}
\widehat{L}^\Lambda \stackrel{\text{def}}{=}\ & (-1)^{\lambda_\alpha+\lambda_\beta+\lambda_\varsigma+\lambda_{\bar\mu}+\lambda_{\bar\nu}+\lambda_{\bar\eta}+1} \sum_{\substack{E_1\Lambda_1\\E_2\Lambda_2}} \big[[W^{E_1}(\lambda_\alpha\lambda_\beta) \times a^{\lambda_\varsigma}]^{\Lambda_1} \times [W^{E_2}(\widetilde{\lambda}_{\bar\mu}\widetilde{\lambda}_{\bar\nu}) \times \tilde{a}^{\lambda_{\bar\eta}}]^{\Lambda_2}\big]^\Lambda \\
& \times (-1)^{\Lambda_1+\Lambda_2}[E_1, E_2, \Lambda_1, \Lambda_2]^{1/2} \sum_{\substack{\Lambda'_1\Lambda'_2\\\Lambda_3\Lambda'}} \sum_{M_3M'} (-1)^{M'}[\Lambda'_1, \Lambda'_2, \Lambda_3, \Lambda']^{1/2} \Omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}(\Lambda'_1\Lambda'_2\Lambda_3\Lambda') \\
& \times \langle \Lambda_3 M_3 \Lambda' - M' | \Lambda M\rangle \begin{Bmatrix} \lambda_\alpha & \lambda_\beta & E_1 \\ \lambda_\varsigma & \Lambda_1 & \Lambda'_1 \end{Bmatrix} \begin{Bmatrix} \lambda_{\bar\mu} & \lambda_{\bar\nu} & E_2 \\ \lambda_{\bar\eta} & \Lambda_2 & \Lambda'_2 \end{Bmatrix} \begin{Bmatrix} \lambda_\alpha & \lambda_{\bar\mu} & \Lambda_3 \\ \Lambda'_1 & \Lambda'_2 & \Lambda' \\ \Lambda_1 & \Lambda_2 & \Lambda \end{Bmatrix}.
\end{aligned} \tag{3.82}$$

The projection-independent $\Omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}(\Lambda'_1\Lambda'_2\Lambda_3\Lambda')$ is defined much the same as the analogous quantity in a two-particle case (see Eq. (3.58)). That is, $\Omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}(\Lambda'_1\Lambda'_2\Lambda_3\Lambda')$ satisfies the equation

$$\begin{aligned}
\omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta} =& (-1)^{\lambda_\alpha+\lambda_\beta+\lambda_\varsigma+\lambda_{\bar\mu}+\lambda_{\bar\nu}+\lambda_{\bar\eta}} \sum_{\Lambda'_1\Lambda'_2} \sum_{\Lambda_3\Lambda'} (-1)^{M'} \langle \lambda_\alpha m_\alpha \lambda_{\bar\mu} - m_{\bar\mu} | \Lambda_3 M_3\rangle \\
& \times E\begin{pmatrix} \lambda_\beta & \lambda_\varsigma & \lambda_{\bar\nu} & \lambda_{\bar\eta} \\ m_\beta & m_\varsigma & -m_{\bar\nu} & -m_{\bar\eta} \end{pmatrix}; \Lambda'_1\Lambda'_2\Lambda' - M'\Big) \Omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}(\Lambda'_1\Lambda'_2\Lambda_3\Lambda').
\end{aligned} \tag{3.83}$$

By a decomposition in Eq. (3.81), the chore to find matrix elements of the three-particle operator $\widehat{L}$ is disintegrated into two distinct tasks: the computation of matrix elements of the irreducible tensor operators $\widehat{\mathcal{O}}^\Lambda([2^21^2]12)$ and the establishment of projection-independent quantities $\Omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}$ that particularly play the role of the effective reduced matrix elements. The latter task depends on a concrete case to be studied. For the expansion terms in the third-order approximation of MBPT, the quantities $\Omega_{\alpha\beta\varsigma\bar\mu\bar\nu\bar\eta}$ are found in Sec. 4 (also, see Appendix C). Conversely, the first task—determination of matrix elements—is independent of the dynamics of system under consideration and thus it can be solved in general.

In Sec. 3.1, the classification of angular reduction schemes of operator string $\widehat{\mathcal{O}}_\ell$, including $\ell = 6$, has been accomplished. The case $\ell = 6$ fits $\widehat{O}_3$ that represents a product of three creation and three annihilation operators (see Eq. (2.42)). A decomposition of $\widehat{\mathcal{O}}_6$ is actualised by Eq. (3.5). Finally, the connection between irreducible tensor operators $\widehat{\mathcal{O}}^\alpha([\lambda]\varkappa)$ is associated by the entries of transformation matrices (Corollary 3.1.4, Definition 3.1.5) $\mathscr{E}$ and $\mathcal{E}^{ij}$. These results are sufficient to find expressions of matrix elements of the sole irreducible tensor operator $\widehat{\mathcal{O}}^\alpha([\lambda]\varkappa)$ associated to a specified angular reduction scheme $\mathscr{T}^{[\lambda]}_\varkappa$: all other matrix elements of the irreducible tensor operators $\widehat{\mathcal{O}}^\alpha([\lambda']\varkappa')$ with $\lambda \neq \lambda'$, $\varkappa \neq \varkappa'$ are found instantly through the transformation coefficients $\mathscr{E}_{\xi\xi'}$ and $\mathcal{E}^{ij}_{\xi'\xi}$. In particular cases, $\mathscr{E}_{\xi\ 14} = \epsilon_\xi$ and $\mathcal{E}^{ij}_{14\ 14} = \varepsilon_{ij}$ take on the values of the basis (Appendix A) and recoupling (Sec. 3.1.3) coefficients. Thus the most natural choice is the scheme $\mathscr{T}_{12}^{[2^21^2]}$.

From now on, the operators $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ that act on the irreducible tensor space $\mathcal{H}^{q}$ will be considered. The notations identified in Sec. 3.1.4 will be used. In the final result, these operators are associated to $\widehat{\mathcal{O}}^{\Lambda}([\lambda]\varkappa)$ acting on $\mathcal{H}^{\Lambda}$ by using Eq. (3.51) for $[\lambda]=[2^21^2]$, $\varkappa=12$. That is,

$$\begin{aligned}
&\big[\lambda^N\Gamma\bar{\Lambda}\|\widehat{\mathcal{O}}^{\Lambda}([2^21^2]12)\|\lambda^N\Gamma'\bar{\Lambda}'\big] = \tfrac{1}{2}\big[\lambda\Gamma Q\bar{\Lambda}|||\widehat{\mathcal{O}}^{0\Lambda}([2^21^2]12)|||\lambda\Gamma' Q\bar{\Lambda}'\big]\\
&+\tfrac{1}{2}\langle Q'M_Q20|QM_Q\rangle\big[\lambda\Gamma Q\bar{\Lambda}|||\widehat{\mathcal{O}}^{2\Lambda}([2^21^2]12)|||\lambda\Gamma' Q'\bar{\Lambda}'\big]\\
&+\tfrac{3}{2\sqrt{5}}\langle Q'M_Q10|QM_Q\rangle\big[\lambda\Gamma Q\bar{\Lambda}|||\widehat{\mathcal{O}}^{1\Lambda}([2^21^2]12)|||\lambda\Gamma' Q'\bar{\Lambda}'\big]\\
&+\tfrac{1}{2\sqrt{5}}\langle Q'M_Q30|QM_Q\rangle\big[\lambda\Gamma Q\bar{\Lambda}|||\widehat{\mathcal{O}}^{3\Lambda}([2^21^2]12)|||\lambda\Gamma' Q'\bar{\Lambda}'\big],
\end{aligned}\tag{3.84}$$

where it is assumed that $\lambda\equiv l^{1}\!/_{2}$ for LS-coupling ($\Lambda\equiv LS$) and $\lambda\equiv j$ for jj-coupling ($\Lambda\equiv J$). The quasispin number $Q={}^{1}\!/_{2}\,(\lambda-v+{}^{1}\!/_{2})$; the basis index $M_Q={}^{1}\!/_{2}\,(N-\lambda-{}^{1}\!/_{2})$. Eq. (3.84) indicates that it is a $\ell=1$–shell case, where the irreps within $\widehat{\mathcal{O}}^{\varsigma}([2^21^2]12)$ (recall that $\alpha\equiv\varsigma\equiv\kappa\Lambda$) satisfy $\alpha_1=\alpha_2=\ldots=\alpha_6=\varsigma_x\equiv{}^{1}\!/_{2}\,\lambda$, where as usually, $x=i,j,k,l,p,q$.

Eq. (3.84) is nothing else but the mathematical realisation of Remark 3.2.1: a one-to-one correspondence for the basis function $|\lambda^N\Gamma\Lambda M\rangle$ of $\mathcal{H}^{\Lambda}$ is the function $|\lambda\Gamma Q\Lambda M_Q M\rangle$ of $\mathcal{H}^{Q}\times\mathcal{H}^{\Lambda}$. It is understood that a particular single-shell case can be extended to $\ell=2,3,4,5,6$. However, in all these cases a correspondence in Eq. (3.51) holds true.

To find the (reduced) matrix element of $\widehat{\mathcal{O}}^{\varsigma}([2^21^2]12)$ that acts on $\ell=2,3,\ldots,6$ electron shells, an efficient preparation of $\widehat{\mathcal{O}}^{\varsigma}([2^21^2]12)$ needs to be established in the same manner as it has been done for the two-particle case. To solve the present task, a classification of operators that act on different number of electron shells is required.

Assuming that the numbers $x\in\{i,j,k,l,p,q\}$ designate the indices of irreps ς_x within $\widehat{\mathcal{O}}^{\varsigma}([2^21^2]12)$ and at the same time they mark the xth electron shell, make the following convenient notations. (In contrast, the index $i=1,2,\ldots,6$ of irrep α_i labels the ith operator a^{α_i} within $\widehat{\mathcal{O}}^{\varsigma}([2^21^2]12)$.)

3.2.4 Definition. The set of operators

$$\widehat{\mathcal{O}}^{\varsigma}([2^21^2]12)\equiv\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)\equiv\big[[W^{\varsigma_{ij}}(\lambda_i\lambda_j)\times a^{\varsigma_k}]^{\varsigma_{ijk}}\times[W^{\varsigma_{lp}}(\lambda_l\lambda_p)\times a^{\varsigma_q}]^{\varsigma_{lpq}}\big]^{\varsigma}\tag{3.85}$$

associated to the angular reduction scheme ($i,j,k,l,p,q\in\mathcal{I}=\{1,2,3,4,5,6\}$)

$$\mathscr{T}_{12}^{[2^21^2]}\equiv\langle ijklpq\rangle\stackrel{\text{def}}{=}\begin{cases}\langle x\rangle, & \text{if } i\le j\le k\le l\le p\le q,\\ \langle x_\pi\rangle, & \text{otherwise,}\end{cases}\tag{3.86}$$

forms the parent class $X_\ell(\Delta_1,\Delta_2,\ldots,\Delta_\ell)$, $\ell\le 6$ of dimension d_ℓ if the subtraction of multiplicities of the same value numbers from the set $s=\{i,j,k\}$ and from the set $s'=\{l,p,q\}$ equals to Δ_x, where

$$\sum_{x=1}^{\ell}\Delta_x=0.\tag{3.87}$$

3.2.5 Definition. The class $X^{*}_{\ell}(\Delta_1,\Delta_2,\ldots,\Delta_\ell)$ of dimension d^{*}_{ℓ} such that

$$X^{*}_{\ell}(\Delta_1,\Delta_2,\ldots,\Delta_\ell)=X_\ell(-\Delta_1,-\Delta_2,\ldots,-\Delta_\ell),\quad d^{*}_{\ell}=d_\ell\tag{3.88}$$

is a dual class.

In other words, the parent class $X_\ell(\Delta_1,\Delta_2,\ldots,\Delta_\ell)$ defines the set of operators $\widehat{\mathcal{O}}^{\varsigma}([2^21^2]12)$ associated to the same angular reduction scheme $\mathscr{T}_{12}^{[2^21^2]}$ but with distinct labelling of irreps so that Eq. (3.87) is valid. The dimension d_ℓ of class equals to the number of such operators.

Example. Suppose there are two operators such that $\alpha_1=\alpha_2=\ldots=\alpha_5=\varsigma_1$, $\alpha_6=\varsigma_2$ for the first one and $\alpha_1=\alpha_2=\alpha_3=\alpha_4=\alpha_6=\varsigma_1$, $\alpha_5=\varsigma_2$ for the second one. Both operators associated to the schemes $\langle 111112\rangle$ and $\langle 111121\rangle$ act on two electron shells. Check the conditions in Eq. (3.87). For the first operator, write $s=\{i=1,j=1,k=1\}$ and $s'=$

$\{l=1,p=1,q=2\}$; the multiplicities of 1 and 2 in s are 3 and 0, respectively. Analogously, the multiplicities of 1 and 2 in s' are 2 and 1. Write $\Delta_1 = 3-2 = +1$, $\Delta_2 = 0-1 = -1$. For the second operator, write $s = \{i=1, j=1, k=1\}$, $s' = \{l=1, p=2, q=1\}$ and $\Delta_1 = 3-2 = +1$, $\Delta_2 = 0-1 = -1$. Then $\Delta_1 + \Delta_2 = +1+(-1) = 0$. Consequently, both operators belong to the same parent class $X_2(+1,-1)$. By Definition 3.2.5, the dual class is $X_2(-1,+1)$, and the operators that correspond to the previous ones are associated to the schemes $\langle 222221\rangle$, $\langle 222212\rangle$.

The choice which class is parent and which one is dual is optional, as it follows from their definitions.

3.2.6 Corollary. *The map*

$$p_\pi\colon\ \langle x\rangle \longrightarrow \langle x_\pi\rangle,\ \begin{pmatrix} i' & j' & k' & l' & p' & q' \\ 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix} \mapsto \begin{pmatrix} i' & j' & k' & l' & p' & q' \\ \pi(1) & \pi(2) & \pi(3) & \pi(4) & \pi(5) & \pi(6) \end{pmatrix} \equiv \begin{pmatrix} i & j & k & l & p & q \\ 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix} \tag{3.89}$$

is realised by

$$\widehat{\pi}\widehat{T}^{\varsigma}(\lambda_{i'}\lambda_{j'}\lambda_{k'}\lambda_{l'}\lambda_{p'}\lambda_{q'}) = \widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q). \tag{3.90}$$

It follows from Corollary 3.2.6 that for $\pi = (ij)$, Eq. (3.90) coincides with Eq. (3.21). In general, the permutation π must be expanded into the product of 2–cycles (transpositions) in order to apply Eq. (3.21) for several times. However, a general solution to count the number of ways in which a given permutation π can be factored into a given number of transpositions (ij) is absent so far. In algebraic combinatorics, authors usually refer to the so-called Hurwitz's formula for the number of minimal transitive factorisations. In a particular case, this formula yields that the number of factorisations of a full cycle in S_ℓ into $\ell-1$ transpositions is $\ell^{\ell-2}$ [94,95]. In Ref. [94], it was also demonstrated that there exists an elegant connection between the primitive factorisation and Jucys–Murphy elements [96–98]. Due to the absence of a general factorisation formula, each permutation π must be expanded in a unique way whenever it appears.

3.2.7 Theorem. *If the operators $\widehat{T}^{\varsigma}(\lambda_{i'}\lambda_{j'}\lambda_{k'}\lambda_{l'}\lambda_{p'}\lambda_{q'})$ and $\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'})$ are associated to the schemes $\langle x\rangle$ and $\langle y\rangle$, and $\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)$, $\widehat{T}^{\varsigma}(\lambda_m\lambda_n\lambda_r\lambda_s\lambda_t\lambda_u)$ are associated to the schemes $\langle x_\pi\rangle$, $\langle y_{\pi'}\rangle$ so that for some $\widehat{\Pi}$, $\widehat{\Pi}\lambda_i = \lambda_m$, $\widehat{\Pi}\lambda_j = \lambda_n$, $\widehat{\Pi}\lambda_k = \lambda_r$, $\widehat{\Pi}\lambda_l = \lambda_s$, $\widehat{\Pi}\lambda_p = \lambda_t$, $\widehat{\Pi}\lambda_q = \lambda_u$, then for the given two maps $p_\pi\colon\ \langle x\rangle \longrightarrow \langle x_\pi\rangle$, $p_{\pi'}\colon\ \langle y\rangle \longrightarrow \langle y_{\pi'}\rangle$, there exists a map $p_{\tilde{\pi}}$ such that the following diagram is commutative*

$$\begin{array}{ccc} \langle y\rangle & \xrightarrow{\ p_{\pi'}\ } & \langle y_{\pi'}\rangle \\ {\scriptstyle p_\pi}\big\downarrow & \nearrow_{p_{\tilde{\pi}}} & \\ \langle y_\pi\rangle & & \end{array} \tag{3.91}$$

and the permutation representation $\widehat{\tilde{\pi}}$ of S_6 is found from

$$\widehat{\tilde{\pi}}\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'}) = \widehat{T}^{\varsigma}(\lambda_{\Pi(i')}\lambda_{\Pi(j')}\lambda_{\Pi(k')}\lambda_{\Pi(l')}\lambda_{\Pi(p')}\lambda_{\Pi(q')}). \tag{3.92}$$

Proof. To prove the theorem, it suffices to demonstrate that the commutator $[\widehat{\pi}, \widehat{\Pi}^{-1}\widehat{\tilde{\pi}}] = 0$, assuming that $\widehat{\Pi}^{-1}\widehat{\Pi} = 1_6$. Indeed, if the latter commutator equals to zero, then, by passing to Eq. (3.92) and the definition of $\widehat{\Pi}$, it is true that $\widehat{\Pi}\widehat{\pi}\widehat{\Pi}^{-1}\widehat{\tilde{\pi}} = \widehat{\pi}' = \widehat{\tilde{\pi}}\widehat{\pi}$ and thus $p_{\pi'} = p_{\tilde{\pi}} \circ p_\pi$.

Find $[\widehat{\pi}, \widehat{\Pi}^{-1}\widehat{\tilde{\pi}}]\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'})$. For $\widehat{\pi}\widehat{\Pi}^{-1}\widehat{\tilde{\pi}}$, write

$$\widehat{\pi}\widehat{\Pi}^{-1}\widehat{\tilde{\pi}}\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'}) = \widehat{\pi}\widehat{\Pi}^{-1}\widehat{T}^{\varsigma}(\lambda_{\Pi(i')}\lambda_{\Pi(j')}\lambda_{\Pi(k')}\lambda_{\Pi(l')}\lambda_{\Pi(p')}\lambda_{\Pi(q')})$$
$$= \widehat{\pi}\widehat{T}^{\varsigma}(\lambda_{i'}\lambda_{j'}\lambda_{k'}\lambda_{l'}\lambda_{p'}\lambda_{q'}) = \widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q).$$

For $\widehat{\Pi}^{-1}\widehat{\tilde{\pi}}\widehat{\pi}$, write

$$\widehat{\Pi}^{-1}\widehat{\tilde{\pi}}\widehat{\pi}\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'}) = \widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)$$

if $[\widehat{\pi}, \widehat{\Pi}^{-1}\widehat{\widetilde{\pi}}] = 0$. Then

$$\widehat{\widetilde{\pi}}\widehat{\pi}\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'}) = \widehat{\Pi}\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q) = \widehat{T}^{\varsigma}(\lambda_m\lambda_n\lambda_r\lambda_s\lambda_t\lambda_u)$$
$$= \widehat{\pi}'\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'})$$

and $\widehat{\pi}' = \widehat{\widetilde{\pi}}\widehat{\pi}$. □

3.2.8 Corollary. *If the operator $\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)$ associated to the scheme $\langle x_\pi\rangle$ belongs to the class $X_\ell(\Delta_1, \Delta_2, \ldots, \Delta_\ell)$ and it is found by realising the map $p_\pi\colon \langle x\rangle \longrightarrow \langle x_\pi\rangle$ for $\widehat{T}^{\varsigma}(\lambda_{i'}\lambda_{j'}\lambda_{k'}\lambda_{l'}\lambda_{p'}\lambda_{q'})$ with $i' \le j' \le k' \le l' \le p' \le q'$, then any other irreducible tensor operator $\widehat{T}^{\varsigma}(\lambda_m\lambda_n\lambda_r\lambda_s\lambda_t\lambda_u) = \widehat{\Pi}\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)$ associated to the scheme $\langle y_{\pi'}\rangle$ of class $X_\ell(\Delta'_1, \Delta'_2, \ldots, \Delta'_\ell)$ is found by realising the map $p_{\pi'} = p_{\widetilde{\pi}} \circ p_\pi$ for $\widehat{T}^{\varsigma}(\lambda_{m'}\lambda_{n'}\lambda_{r'}\lambda_{s'}\lambda_{t'}\lambda_{u'})$ with $m' \le n' \le r' \le s' \le t' \le u'$, where $\widehat{\widetilde{\pi}}$ is found from Eq. (3.92). The class $X_\ell(\Delta'_1, \Delta'_2, \ldots, \Delta'_\ell)$ is called the derived class of dimension d_ℓ.*

Proof. By Definition 3.2.4, the proof is similar to the one applied to Theorem 3.2.7. □

3.2.9 Corollary. *The dual class $X^*_\ell(\Delta_1, \Delta_2, \ldots, \Delta_\ell)$ is a particular case of the derived class $X_\ell(\Delta'_1, \Delta'_2, \ldots, \Delta'_\ell)$ if $\Delta'_1 = -\Delta_1, \Delta'_2 = -\Delta_2, \ldots, \Delta'_\ell = -\Delta_\ell$; each derived class has its dual one which is of the same dimension.*

Corollary 3.2.9 indicates that for a given parent class, all three types of classes—parent, dual, derived—are of the identical dimension.

Theorem 3.2.7 allows us to reduce the number of classes that need to be studied to classify the irreducible tensor operators which act on $\ell = 2, 3, \ldots, 6$ electron shells. The classification of all the rest operators that belong to the corresponding derived class is performed immediately by using Eq. (3.91), once the permutation representation $\widehat{\widetilde{\pi}}$ is found. In addition, it ought to be by no means obvious that Theorem 3.1.8 also fits Eq. (3.90), thus the permutations that arise during the transformations are «simplified», as it can be recognised from the tables in Appendix B.

In Tabs. 20-35 (Appendix B), the dual classes are not listed. The reason for not doing so is simple. If the operator $\widehat{L}$ expanded by using Eq. (3.81) belongs to the parent class $X_\ell(\Delta_1, \Delta_2, \ldots, \Delta_\ell)$, then its adjoint operator $\widehat{L}^\dagger$ belongs to the dual class $X^*_\ell(\Delta_1, \Delta_2, \ldots, \Delta_\ell)$ which is nothing else but $X_\ell(-\Delta_1, -\Delta_2, \ldots, -\Delta_\ell)$ (Definition 3.2.5). Consequently, the matrix element $\langle\Psi_i|\widehat{L}^\dagger|\Psi_j\rangle$ on the basis given in Eq. (2.2) simply equals to the matrix element $\langle\Psi_j|\widehat{L}|\Psi_i\rangle$ if recalling that the matrix element on the infinite-dimensional N–electron Hilbert space $\mathcal{H}$ is defined by the map $X \times X \longrightarrow \mathbb{R}$, where X denotes the set of basis Ψ_i (Sec. 2.1). The similar argument holds for the dual classes $X^*_\ell(\Delta'_1, \Delta'_2, \ldots, \Delta'_\ell)$ associated to the derived classes $X_\ell(\Delta'_1, \Delta'_2, \ldots, \Delta'_\ell)$. Thus, the only task is to identify a given irreducible tensor operator $T^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)$ by using Definition 3.2.4. This is easily done utilising Tabs. 36-39 in Appendix B. For a particular two-shell case, the identification of operators is trivial: there are only parent and derived classes; the derived classes coincide with the dual ones.

Example (Operator identification). Consider operator $\widehat{T}^{\varsigma}(\lambda_5\lambda_3\lambda_2\lambda_4\lambda_1\lambda_4)$ associated to the angular reduction scheme $\langle 532414\rangle$. This is a 5–shell case. Find the associated class. By Definition 3.2.4, write $s = \{i = 5, j = 3, k = 2\}$, $s' = \{l = 4, p = 1, q = 4\}$: $\Delta_1 = 0 - 1 = -1$, $\Delta_2 = 1 - 0 = 1$, $\Delta_3 = 1 - 0 = 1$, $\Delta_4 = 0 - 2 = -2$, $\Delta_5 = 1 - 0 = 1$. The condition $\sum_{x=1}^{5} \Delta_x = 0$ is satisfied, thus the operator belongs to the class $X_5(-1, +1, +1, -2, +1)$. Identify the class in Tab. 38 (Appendix B). The present class is the dual class of $X_5(+1, -1, -1, +2, -1)$ which is the derived class associated to the parent class $X_5(+2, +1, -1, -1, -1)$. This implies that the matrix element of $\widehat{L} \propto \sum a_5 a_3 a_2 a_4^\dagger a_1^\dagger a_4^\dagger$ (see Eq. (3.80)) is equal to the matrix element of $\widehat{L}' \propto \sum a_4 a_1 a_4 a_2^\dagger a_3^\dagger a_5^\dagger$, where $\widehat{L}^\dagger = \widehat{L}'$. Consequently, the operator $\widehat{T}^{\varsigma}(\lambda_4\lambda_1\lambda_4\lambda_2\lambda_3\lambda_5)$ of the derived class $X_5(+1, -1, -1, +2, -1)$ must be studied. Refer to Tab. 33. Since $\langle y_{\pi'}\rangle = \langle 414235\rangle$ and $\langle y\rangle = \langle 123445\rangle$, $\pi' = (142)(35)$, where $(142) = (12)(14)$. By Eq. (3.21),

$$\widehat{\pi}'\widehat{T}^{\varsigma}(\lambda_1\lambda_2\lambda_3\lambda_4\lambda_4\lambda_5) = \widehat{T}^{\varsigma}(\lambda_4\lambda_1\lambda_4\lambda_2\lambda_3\lambda_5) = \sum_{\substack{\varsigma_{12}\varsigma_{123}\\ \varsigma_{44}\varsigma_{445}}} \varepsilon_{\pi'}\, \widehat{T}^{\varsigma}(\lambda_1\lambda_2\lambda_3\lambda_4\lambda_4\lambda_5),$$

$$\varepsilon_{\pi'} = \sum_{\varsigma_{24}\varsigma_{134}\varsigma_{245}} \varepsilon_{(142)(35)}\varepsilon_{(12)(14)}\varepsilon_{12}.$$

Other 17 operators that belong to the derived class $X_5(+1,-1,-1,+2,-1)$ are obtained making use of Eq. (3.91) for $\tilde{\pi} = (153)(24)$.

Tab. 7: The parameters for three-particle matrix elements: $\ell = 2$

$X_2\,(\Delta_1,\Delta_2)$	$\langle x\rangle$	ξ	w_1	w_2
$X_2\,(0,0)$	$\langle 111122\rangle$	20	1111	22
	$\langle 112222\rangle$	5	2222	–
	$\langle 111112\rangle$	27	1111	11111
$X_2\,(+1,-1)$	$\langle 111222\rangle$	14	–	–
	$\langle 122222\rangle$	30	2222	22222

Tab. 8: The parameters for three-particle matrix elements: $\ell = 3$

$X_3\,(\Delta_1,\Delta_2,\Delta_3)$	$\langle x\rangle$	ξ	w_1	w_2	w_3
$X_3\,(0,0,0)$	$\langle 112233\rangle$	1	22	33	1122
	$\langle 111123\rangle$	27	1111	11112	–
$X_3\,(+2,-1,-1)$	$\langle 112223\rangle$	4	222	11222	–
	$\langle 112333\rangle$	14	–	–	–
$X_3\,(+3,-2,-1)$	$\langle 111223\rangle$	15	11122	–	–
	$\langle 123333\rangle$	5	3333	–	–
$X_3\,(+1,-1,0)$	$\langle 111233\rangle$	20	1112	33	–
	$\langle 122233\rangle$	24	22	33	222
Derived class	$\langle y\rangle$				
$X_3\,(-1,+2,-1)$	$\langle 122223\rangle$	31	222	2222	12222
	$\langle 122333\rangle$	6	22	–	–

Tab. 9: The parameters for three-particle matrix elements: $\ell = 4$

$X_4\,(\Delta_1,\Delta_2,\Delta_3,\Delta_4)$	$\langle x\rangle$	ξ	w_1	w_2	w_3
$X_4\,(+1,+1,-1,-1)$	$\langle 111234\rangle$	27	1112	11123	–
	$\langle 122234\rangle$	29	222	1222	12223
	$\langle 123334\rangle$	4	333	12333	–
	$\langle 123444\rangle$	14	–	–	–
$X_4\,(+2,-2,+1,-1)$	$\langle 112234\rangle$	3	22	1122	11223
Derived classes	$\langle y\rangle$				
$X_4\,(+2,+1,-2,-1)$	$\langle 112334\rangle$	15	11233	–	–
$X_4\,(+2,+1,-1,-2)$	$\langle 112344\rangle$	20	44	1123	–
$X_4\,(+1,+2,-2,-1)$	$\langle 122334\rangle$	7	12233	–	–
$X_4\,(+1,+2,-1,-2)$	$\langle 122344\rangle$	23	44	1223	–
$X_4\,(+1,-1,+2,-2)$	$\langle 123344\rangle$	1	33	44	1233

Tab. 10: The parameters for three-particle matrix elements: $\ell = 5$

$X_5\,(\Delta_1,\Delta_2,\Delta_3,\Delta_4,\Delta_5)$	$\langle x\rangle$	ξ	w_1	w_2	w_3
$X_5\,(+2,+1,-1,-1,-1)$	$\langle 112345\rangle$	27	1123	11234	–
$X_5\,(+1,+1,-1,-1,0)$	$\langle 123455\rangle$	20	55	1234	–
Derived classes	$\langle y\rangle$				
$X_5\,(+1,+2,-1,-1,-1)$	$\langle 122345\rangle$	28	22	1223	12234
$X_5\,(-1,-1,+2,+1,-1)$	$\langle 123345\rangle$	3	33	1233	12334
$X_5\,(-1,+1,-1,+2,-1)$	$\langle 123445\rangle$	15	12344	–	–

To conclude, a general formula of reduced matrix element of $\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)$ is displayed assuming that $\ell > 1$ and $i \le j \le k \le l \le p \le q$.

$$\left[(\lambda_1+\lambda_2+\ldots+\lambda_\ell)\Gamma_1 q_1\Gamma_2 q_2 q_{12}\ldots\Gamma_\ell q_\ell q|||\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)|||(\lambda_1+\lambda_2+\ldots+\lambda_\ell)\right.$$
$$\left.\bar{\Gamma}_1\bar{q}_1\bar{\Gamma}_2\bar{q}_2\bar{q}_{12}\ldots\bar{\Gamma}_\ell\bar{q}_\ell\bar{q}\right] = (-1)^{\Phi_\ell}\sum_{\varsigma_w\in\mathcal{L}_\xi}\epsilon_\xi\prod_{x=1}^{\ell}[q_{12\ldots x},q_{x+1},\bar{q}_{12\ldots x+1},\varsigma_{p_x+1}]^{1/2}$$
$$\times\left[\lambda_x\Gamma_x q_x|||\widehat{U}^{\varsigma_{p_{xx}}}(\lambda_x\lambda_x\ldots\lambda_x)|||\lambda_x\bar{\Gamma}_x\bar{q}_x\right]\begin{Bmatrix}\bar{q}_{12\ldots x} & \bar{q}_{x+1} & \bar{q}_{12\ldots x+1}\\ \varsigma_{p_x} & \varsigma_{p_{x+1}\,x+1} & \varsigma_{p_{x+1}}\\ q_{12\ldots x} & q_{x+1} & q_{12\ldots x+1}\end{Bmatrix}, \tag{3.93}$$

where $q\equiv Q\Lambda$, $q_{12\ldots\ell}=q$, $\bar{q}_{12\ldots\ell}=\bar{q}$, $\varsigma_{p_\ell}=\varsigma$. In Eq. (3.93), the $\mathcal{N}_x$–length numbers $p_x=11\ldots122\ldots2xx\ldots x$, $p_{xx}=xx\ldots x$, where $\mathcal{N}_x$ is the multiplicity of equal irreps ς_x within $\widehat{T}^{\varsigma}(\lambda_i\lambda_j\lambda_k\lambda_l\lambda_p\lambda_q)$. The phase multiplier

$$\Phi_\ell\stackrel{\text{def}}{=}\sum_{x=1}^{\ell}\Big((N_x+\mathcal{N}_x+\Delta_x)\sum_{y>x}^{\ell}N_y+\mathcal{N}_x\sum_{z=1}^{x-1}(N_z+\Delta_z)\Big). \tag{3.94}$$

N_x denotes the number of electrons in the shell characterised by the numbers $\lambda_x\Gamma_x Q_x\Lambda_x M_{Q_x}M_x$; $M_{Q_x}=1/2\,(N_x-\lambda_x-1/2)$; Δ_x is recognised from the class that contains a given irreducible tensor operator. The indices of summation $w\in\mathcal{L}_\xi=\{w_1,w_2,w_3\}$ depend on a specified operator. Possible values are listed in Tabs. 7-10. Particularly for $\ell=6$, $\xi=27$, $w_1=1234$, $w_2=12345$, w_3 is absent.

The operator $\widehat{U}^{\varsigma_{p_{xx}}}(\lambda_x\lambda_x\ldots\lambda_x)$ is associated to the angular reduction schemes: $\mathscr{T}_1^{[1^2]}$ for $\mathcal{N}_x=2$; $\mathscr{T}_2^{[21]}$ for $\mathcal{N}_x=3$; $\mathscr{T}_1^{[21^2]}$ for $\mathcal{N}_x=4$; $\mathscr{T}_1^{[21^3]}$ for $\mathcal{N}_x=5$; $\mathscr{T}_{12}^{[2^21^2]}$ for $\mathcal{N}_x=6$. The reduced matrix elements of $\widehat{U}^{\Lambda}$ on $\mathcal{H}^{\Lambda}$ are known [54, Eq. (25)]. Thus the connection with $\widehat{U}^{\varsigma}$ is actualised making use of Tab. 6 and Eq. (3.51) which fits the case $\mathcal{N}_x=6$ (see also Eq. (3.84)).

3.3 Summary and concluding remarks

Theoretical atomic physics deals with various irreducible tensor operators that allow us to account for the contribution of atomic as well as effective interactions in a simplified form: the irreducible tensor operators attach the symmetry properties of atom. In mathematical formulation, the contributions are evaluated by calculating matrix elements – the real scalar products on the many-electron Hilbert spaces. In practice, the calculation of matrix elements on the basis of many-electron wave functions is a very complicated task. The reason for this is a complex tensor structure of many-electron operators. The one-electron and two-electron operators that are most common in atomic physics are examined very well. In contrast, the study of triple or even higher excitations is already troublesome and an uncertain one so far. Due to a complexity, it has become standard in many cases of MBPT to account for the contributions of single or double excitations only. But the approximation stipulates the physical problems that can be solved theoretically. On the other hand, the practice requires a more valued precision. The best example is the atomic parity violation [42, 57], the study of which is a very popular task among the atomists nowadays: the contribution of at least triple excitations becomes inevitable. Therefore in most cases, Sec. 3 is concentrated on the present problem.

Sec. 3.1.1 provides an opportunity to classify the angular reduction schemes of operator string $\widehat{\mathcal{O}}_\ell$ (see Eq. (3.1)) for any integer ℓ. The classification is performed by using: the ℓ–numbers (Definition 3.1.1), the S_ℓ–irreducible representations $[\lambda]$, the ℓ_2–tuples. The idea—in its most general form—is simple: every angular reduction scheme is characterised by the irrep $[\lambda]$, thus making the restriction (items I-III in Sec. 3.1.1) $\mathrm{S}_\ell\to\mathrm{S}_{\ell'}\to\ldots\to\mathrm{S}_{\ell''}$ until $\ell''\le 3$, a given complex structure associated to $[\lambda]$ is transformed to the scheme associated to either $[21]$ or $[1^2]$ (Tabs. 3-4). The path of such a restriction is therefore a unique angular reduction scheme.

Sec. 3.1.2 concentrates on the case $\ell=6$ which characterises the three-particle operators. The correspondence of angular reduction schemes (42 in total) is actualised by using the entries $\mathscr{E}_{\xi\xi'}$, $\xi,\xi'=1,2,\ldots,42$ of a 42×42 transformation matrix $\mathscr{E}$ (Corollary 3.1.4). These entries are constructed from the so-called basis coefficients ϵ_ξ that relate operators associated to the

scheme $\mathscr{T}^{[2^2 1^2]}_{12}$ with all the rest operators that are constructed by using different schemes $\mathscr{T}^{[\lambda]}_{\varkappa}$ (refer to Eq. (3.11)). The basis coefficients are displayed in Appendix A.

In Sec. 3.1.3, the permutation properties of the irreps within a given operator $\widehat{\mathcal{O}}^{\alpha}([\lambda]\varkappa)$ associated to the angular reduction scheme $\mathscr{T}^{[\lambda]}_{\varkappa}$ are studied for $\ell = 6$. The symmetry group S_6 contains $6!$ permutations at all. However, each permutation or a product of permutations is a product of transpositions whose total number is 15 (see Eq. (3.19)). Thus the task that deals with operators with different ordering of irreps is confined to the task to find the transformation coefficients $\mathcal{E}^{ij}_{\xi'\xi}$ (Definition 3.1.5) formed from the so-called recoupling coefficients ε_{ij} (see Eq. (3.21)). These coefficients relate operators constructed by using the ordering $(\alpha_1, \alpha_2, \ldots, \alpha_6)$ with the operators constructed by using the ordering $(\alpha_{\pi(1)}, \alpha_{\pi(2)}, \ldots, \alpha_{\pi(6)})$, where $\pi \in \mathrm{S}_6$ is a transposition. The expressions of ε_{ij} are found by making use of the so-called commutative diagrams (see Eq. (3.30)). The originated method based on Eq. (3.29) allows us to find the recoupling coefficients by making the least number of transformations that are required by the permutation representation $\widehat{\pi}$. Consequently, it reduces the number of intermediate irreps.

Sec. 3.1.4 is a very important addition to the method presented in Sec. 3.1.3. The main idea is listed in Theorem 3.1.8 which is, again, a statement that allows us to reduce the number of indices of summation. Meanwhile, the present theorem is one of the key features that stipulate the further on foundation of the simplification of classification of the three-particle operators acting on many-electron shells (Appendix B).

In Sec. 3.2, the irreducible tensor operators associated to some special angular reduction schemes are considered. For the two-particle case (Sec. 3.2.1), the most common schemes are $\mathscr{T}^{[2^2]}_{1}$ and $(\widehat{\pi}_{243}\mathscr{T})^{[2^2]}_{1}$ which are also known [77] as the z-scheme and b-scheme, respectively. The b-scheme first originated by Kaniauskas [85] is the most typical one. However, in Sec. 4, the advantage of a less common z-scheme will be demonstrated.

Finally, Sec. 3.2.2 demonstrates the method to classify the three-particle operators that act on $\ell = 2, 3, 4, 5, 6$ electron shells. The algorithm is based on Theorem 3.2.7; the realisation – on Theorem 3.1.8. The operators are grouped into the three types of classes: parent, dual, derived (Definition 3.2.4, Definition 3.2.5, Corollary 3.2.8). The identification of operators that belong to a specified class is performed making use of the tables in Appendix B. The present identification makes it possible to calculate the matrix elements of three-particle operators efficiently: the tables of classes display the relationship between the operators that belong to the parent class and the operators that belong to the derived classes. Thus it suffices to find the expression of matrix element (see Eq. (3.93)) for the sole operator – the matrix elements of other operators are found instantly.

In Sec. 2.3, a general expression of the Fock space operator has been presented (refer to Eq. (2.41)). In Sec. 2.3.1, its confinement on the many-electron Hilbert space has been obtained (to compare with, see Eqs. (2.55), (2.59)) leading to Lemma 2.3.9 and Theorem 2.3.12. As a result, Eq. (2.69) has been derived for the n–body parts ($n = 1, 2, 3, 4$) of wave operator that is necessary to compute the terms of effective Hamiltonian in Eq. (2.61). Based on the methods, developed in the present section, it is now possible to form the irreducible tensor operators of both the wave operator and the effective Hamiltonian in a systematic way. However, still one more problem remains unsolved. This is the n–body effective matrix element ω_n (see Eq. (2.65)). As already pointed out in Sec. 3.2, these elements are related to a specified system under consideration. In the next section, the terms of the third-order MBPT ($k = 2$ in Eq. (2.71)) will be considered and the n–body ($n = 1, 2, 3, 4$) effective matrix elements of the kth–order ($k = 1, 2, 3$) will be displayed expressly.

4 Applications to the third-order MBPT

The main goal of the present section is a symbolic preparation of terms of the third-order effective Hamiltonian $\widehat{\mathscr{H}}^{(3)}$ so that the expressions attach an applicability to the coupled-cluster (CC) approach as well.

To bring the purpose to a successful end, two tasks are to be solved: the generation of expansion terms and their appropriation.

The generation of terms is related to the selection of model space in open-shell MBPT. The model space $\mathcal{P}$ has been selected in Sec. 2.3 (also, see Definition 2.3.2 and Corollary 2.3.3). To generate the terms of $\widehat{\mathscr{H}}^{(3)}$, the n–body parts of $\widehat{\Omega}^{(1)}$ and $\widehat{\Omega}^{(2)}$ are required (see Eqs. (2.61), (2.71)). These are found from the generalised Bloch equation (refer to Eqs. (2.58), (2.59))

$$[\widehat{\Omega}^{(1)}, \widehat{H}_0]\widehat{P} = \widehat{Q}(\widehat{V}_1 + \widehat{V}_2)\widehat{P}, \quad \widehat{\Omega}^{(1)} = \sum_{n=1}^{2} \widehat{\Omega}^{(1)}_n, \tag{4.1}$$

$$[\widehat{\Omega}^{(2)}, \widehat{H}_0]\widehat{P} = \widehat{Q}(\widehat{V}_1 + \widehat{V}_2)\widehat{\Omega}^{(1)}\widehat{P}, \quad \widehat{\Omega}^{(2)} = \sum_{n=1}^{4} \widehat{\Omega}^{(2)}_n. \tag{4.2}$$

The solutions for $\widehat{\Omega}^{(k)}_n$ are of the form given by Eq. (2.69) replacing ω with $\omega^{(k)}$. Then the third-order contribution to $\widehat{\mathscr{H}}$ reads (see Eq. (2.66))

$$\widehat{\mathscr{H}}^{(3)} = \sum_{I_{m+n-\xi}} \sum_{m=1}^{2} \sum_{n=1}^{4} \sum_{\xi=1}^{\min(2m,2n)} \widehat{h}^{(3)}_{mn;\xi}, \quad \widehat{h}^{(3)}_{mn;\xi} \stackrel{\text{def}}{=} :\{\widehat{P}\widehat{V}_m\widehat{\Omega}^{(2)}_n\widehat{P}\}_\xi:, \tag{4.3}$$

where $\widehat{h}^{(3)}_{mn;\xi}$, the $(m+n-\xi)$–body operator (Tab. 11), must be expanded into the sum of irreducible tensor operators. The confinement of the space the operator acts on is the second task to be solved. A common technique of expansion of N–electron model space $\mathcal{P}$ into the orthogonal sum of its $\mathrm{SU}(2)$–irreducible subspaces $\mathcal{P}^\Lambda$ leads to

$$\widehat{h}^{(3)}_{mn;\xi} = \sum_{\Lambda} \sum_{M=-\Lambda}^{+\Lambda} \sum_{\Gamma} \widehat{O}^\Lambda_M([\lambda]\varkappa)\, \mathfrak{h}^{(3)}_{mn;\xi}(\Gamma\Lambda). \tag{4.4}$$

Tab. 11: Possible values of m, n, ξ necessary to build the $(m+n-\xi)$–body terms of $\widehat{\mathscr{H}}^{(3)}$

$m+n-\xi$	m	n	ξ	$m+n-\xi$	m	n	ξ	$m+n-\xi$	m	n	ξ
0	1	1	2	2	2	1	1	3	1	3	1
	2	2	4		1	2	1		2	3	2
1	1	1	1		2	2	2		1	4	2
	2	1	2		1	3	2		2	4	3
	1	2	2		2	3	3	4	2	3	1
	2	2	3		2	4	4		1	4	1
	2	3	4	3	2	2	1		2	4	2
								5	2	4	1

By Lemma 2.3.9, the irreducible tensor operator $\widehat{O}^\Lambda([\lambda]\varkappa)$ associated to the angular reduction scheme $\mathscr{T}^{[\lambda]}_\varkappa$ contains creation and transposed annihilation operators labelling the valence states only. As usually, Γ denotes additional numbers that are necessary to characterise studied operators. $\mathfrak{h}^{(3)}_{mn;\xi}(\Gamma\Lambda)$ denotes the projection-independent coefficient; thus it is the $\mathrm{SU}(2)$–invariant. At this step, it should be pointed out the two principal differences to compare with the traditional version of MBPT, though they are easily seen from Eqs. (2.69), (4.2), (4.4). These differences, however, comprise their own benefits that are the key features of the method presented here.

1. The generalised Bloch equation for $\widehat{\Omega}^{(k)}$ indicates that the solutions are proportional to the kth power of perturbation $\widehat{V}$. For instance, $\widehat{\Omega}^{(1)} \propto \widehat{V}$ (see Eq. (4.1)), $\widehat{\Omega}^{(2)} \propto \widehat{V}\widehat{\Omega}^{(1)} \propto \widehat{V}^2$

(see Eq. (4.2)), etc. This is also true for the terms of effective Hamiltonian (see Eq. (4.3)): $\widehat{\mathscr{H}}^{(3)} \propto \widehat{V}\widehat{\Omega}^{(2)} \propto \widehat{V}^3$, etc. Each m–body part of perturbation $\widehat{V}$ (refer to Eqs. (2.40)-(2.43)) contains the m–body matrix element $v_m(\alpha\bar{\beta})$. Consequently, $\widehat{\Omega}^{(k)}$ contains the product of k such elements. Moreover, every single term in $\widehat{\Omega}^{(k)}$—obtained by using the Wick's theorem—is evaluated separately. A typical example is the classical work of Ho et. al. [37]. (The latter method of evaluation did not change until nowadays.) It should be obvious that such interpretation becomes tedious when a huge number of diagrams is generated. This fact makes sense especially for the higher-order PT. In the present case, on the other hand, the solutions for $\widehat{\Omega}^{(k)}$ are given by Eq. (2.69) with a single element $\omega^{(k)}$. Thus $\omega^{(k)}$ represents the product of k matrix elements of $\widehat{V}_m$ with energy denominators included. In other words, $\omega_n^{(k)}$ is the kth–order n–body effective matrix element that characterises the n–body part of the kth–order wave operator. In addition to the convenience of otherwise marked product of matrix elements v_m, there is also an essential peculiarity: by Theorem 2.3.12, the terms of $\widehat{\Omega}^{(k)}$ are combined in groups (refer to Eq. (2.69)) related to the different types (core, valence, excited) of single-electron orbitals. That is, a number of Golstone diagrams drawn in $\omega^{(k)}$ are characterised by the sole tensor structure and thus the problem of evaluation of each separate diagram is eliminated. Meanwhile, in CC approach, the n–particle effects are embodied in the so-called amplitudes ρ_n (see, for example, Ref. [42]) of excitation that are, in principal, the n–body effective matrix elements. Therefore, if replacing $\omega_n^{(k)}$ with ρ_n, the tensor structure of terms remains steady and thus such formulation is applicable to at least two approaches of PT.

2. In traditional MBPT, the two-particle matrix elements $v_2(\alpha\bar{\beta})$ or else $g_{\alpha\beta\bar{\mu}\bar{\nu}}$ (see Eq. (3.53)) are expressed in terms of b-coefficient (Sec. 3.2.1). In this case, as it will be confirmed later, a z-scheme is preferred.

4.1 The treatment of terms of the second-order wave operator

The generation of expansion terms of $\widehat{\Omega}^{(2)}$ is clearly a computational task and it is the most time consuming process. The nowadays software programs are capable to solve the problems of the present type. To generate the terms, the symbolic package *NCoperators* written on *Mathematica* is used. The features of the package are studied in a more detail in Appendix D, while in the present section, the study of already generated terms is argued.

Despite of a large number of generated terms of $\widehat{\Omega}^{(2)}$, fortunately, there are only a few of fundamental constructions that need to be considered: all the rest terms are obtained varying the known expressions.

In total, there are 13 such constructions (Tabs. 12-14). In tables, $g_{\alpha\beta\bar{\mu}\bar{\nu}}$ and $\widetilde{g}_{\alpha\beta\bar{\mu}\bar{\nu}}$, the matrix representations of a two-particle interaction operator g_{12}, are defined by Eqs. (3.53)-(3.54). Their explicit expressions are found from Eqs. (3.63)-(3.64). For the typical interaction operators g_{12} observed in atomic physics, the expressions of z coefficients are listed in the examples of Sec. 3.2.1. Here, Remark 3.2.3 is taken into account. The single-particle matrix representation $v_{\alpha\bar{\beta}}$ of the self-adjoint interaction operator v_i reads (refer to Eq. (2.43))

$$v_{\alpha\bar{\beta}} = v_{\bar{\beta}\alpha} \stackrel{\text{def}}{=} \langle\alpha|v_i|\bar{\beta}\rangle = (-1)^{\lambda_{\bar{\beta}}+m_{\bar{\beta}}} f(\tau_i\lambda_\alpha\lambda_{\bar{\beta}})\langle\lambda_\alpha m_\alpha \lambda_{\bar{\beta}} - m_{\bar{\beta}}|\tau_i m_i\rangle, \tag{4.5}$$

$$f(\tau_i\lambda_\alpha\lambda_{\bar{\beta}}) \stackrel{\text{def}}{=} -\frac{[\lambda_\alpha]^{1/2}}{[\tau_i]^{1/2}}\big[n_\alpha\lambda_\alpha\|v^{\tau_i}\|n_{\bar{\beta}}\lambda_{\bar{\beta}}\big]. \tag{4.6}$$

In Eqs. (4.5)-(4.6), v^{τ_i} denotes the $\mathrm{SO}(3)$–irreducible tensor operator that acts on the subspace of the space the operator v_i acts on. It is assumed that the single-particle Slater integral(s) is involved in $f(\tau_i\lambda_\alpha\lambda_{\bar{\beta}})$. The number of such integrals depends on the basis $|n_\alpha\lambda_\alpha m_\alpha\rangle$. The numbers $f(\tau_i\lambda_\alpha\lambda_{\bar{\beta}})$ are complex, in general, and they satisfy

$$\overline{f(\tau_i\lambda_{\bar{\beta}}\lambda_\alpha)} = o(\tau_i\lambda_\alpha\lambda_{\bar{\beta}})f(\tau_i\lambda_\alpha\lambda_{\bar{\beta}}), \tag{4.7}$$

Tab. 12: The multipliers for one-particle effective matrix elements of $\widehat{\Omega}^{(2)}$

Construction	SU(2)–invariant: Expression
$\sum_{\mu} v_{\alpha\mu}\omega^{(1)}_{\mu\bar{\beta}}$	$S_{\alpha\bar{\beta}}(\tau_1\tau_2\tau)$: $(-1)^{\lambda_{\bar{\beta}}-\lambda_\alpha-\tau}[\tau_1,\tau_2]^{1/2}\sum_{\mu}\frac{f(\tau_1\lambda_\alpha\lambda_\mu)f(\tau_2\lambda_\mu\lambda_{\bar{\beta}})}{\varepsilon_{\bar{\beta}}-\varepsilon_\mu}\begin{Bmatrix}\tau_1 & \tau_2 & \tau\\ \lambda_{\bar{\beta}} & \lambda_\alpha & \lambda_\mu\end{Bmatrix}$ $\times\langle\tau_1 m_1\tau_2 m_2|\tau m\rangle$
$\sum_{\zeta\bar{\mu}} v_{\zeta\bar{\mu}}\widetilde{\omega}^{(1)}_{\bar{\mu}\alpha\zeta\bar{\beta}}$	$\widetilde{S}_{\alpha\bar{\beta}}(\tau_1)$: $2(-1)^{\lambda_\alpha+\lambda_{\bar{\beta}}}\sum_{\zeta\bar{\mu}}(-1)^{\lambda_\zeta+\lambda_{\bar{\mu}}}\frac{f(\tau_1\lambda_\zeta\lambda_{\bar{\mu}})}{\varepsilon_{\zeta\bar{\beta}}-\varepsilon_{\alpha\bar{\mu}}}\sum_u[u]^{1/2}\begin{Bmatrix}\tau_1 & \lambda_\zeta & \lambda_{\bar{\mu}}\\ u & \lambda_\alpha & \lambda_{\bar{\beta}}\end{Bmatrix}$ $\times\widetilde{z}(0\lambda_{\bar{\mu}}\lambda_\alpha\lambda_{\bar{\beta}}\lambda_\zeta uu)$
$\sum_{\zeta\bar{\mu}}\widetilde{g}_{\bar{\mu}\alpha\zeta\bar{\beta}}\omega^{(1)}_{\zeta\bar{\mu}}$	$\widetilde{S'}_{\alpha\bar{\beta}}(\tau_2)$: $\widehat{R}\left(\begin{smallmatrix}\bar{\beta}\zeta\to\bar{\mu}\\ \alpha\bar{\mu}\to\zeta\end{smallmatrix}\right)\widetilde{S}_{\alpha\bar{\beta}}(\tau_2)$
$\sum_{\rho\eta\zeta}\widetilde{g}_{\alpha\zeta\rho\eta}\widetilde{\omega}^{(1)}_{\rho\eta\zeta\bar{\beta}}$	$\widetilde{S}_{\alpha\bar{\beta}}$: $4\delta_{\lambda_\alpha\lambda_{\bar{\beta}}}[\lambda_\alpha]^{-1/2}\sum_u\sum_{\rho\eta\zeta}(-1)^{\lambda_\rho-\lambda_\eta-u}\frac{1}{\varepsilon_{\bar{\beta}\zeta}-\varepsilon_{\rho\eta}}$ $\times\widetilde{z}(0\lambda_\alpha\lambda_\zeta\lambda_\eta\lambda_\rho uu)\widetilde{z}(0\lambda_\rho\lambda_\eta\lambda_\alpha\lambda_\zeta uu)$

Tab. 13: The multipliers for two-particle effective matrix elements of $\widehat{\Omega}^{(2)}$

Construction	SU(2)–invariant: Expression
$v_{\alpha\bar{\mu}}\omega^{(1)}_{\beta\bar{\nu}}$	$D_{\alpha\beta\bar{\mu}\bar{\nu}}(ud\tau)$: $[\tau_1,\tau_2,u,d]^{1/2}\frac{f(\tau_1\lambda_\alpha\lambda_{\bar{\mu}})f(\tau_2\lambda_\beta\lambda_{\bar{\nu}})}{\varepsilon_{\bar{\nu}}-\varepsilon_\beta}\langle\tau_1 m_1\tau_2 m_2|\tau m\rangle$ $\times\begin{Bmatrix}\lambda_\alpha & \lambda_\beta & u\\ \lambda_{\bar{\mu}} & \lambda_{\bar{\nu}} & d\\ \tau_1 & \tau_2 & \tau\end{Bmatrix}$
$\sum_{\zeta} v_{\alpha\zeta}\omega^{(1)}_{\zeta\beta\bar{\mu}\bar{\nu}}$	$D_{\alpha\beta\bar{\mu}\bar{\nu}}(Uu\tau_1)$: $2(-1)^{\lambda_\alpha-\lambda_\beta+\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+\tau_1}[U]^{1/2}\sum_{\zeta}\frac{f(\tau_1\lambda_\alpha\lambda_\zeta)}{\varepsilon_{\bar{\mu}\bar{\nu}}-\varepsilon_{\beta\zeta}}z(0\lambda_\zeta\lambda_\beta\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}uu)$ $\times\begin{Bmatrix}\tau_1 & \lambda_\alpha & \lambda_\zeta\\ \lambda_\beta & u & U\end{Bmatrix}$
$\sum_{\zeta} g_{\zeta\beta\bar{\mu}\bar{\nu}}\omega^{(1)}_{\alpha\zeta}$	$D'_{\alpha\beta\bar{\mu}\bar{\nu}}(Uu\tau_2)$: $\widehat{R}\left(\begin{smallmatrix}\bar{\mu}\bar{\nu}\to\zeta\\ \beta\zeta\to\alpha\end{smallmatrix}\right)D_{\alpha\beta\bar{\mu}\bar{\nu}}(Uu\tau_2)$
$\sum_{\zeta\rho} g_{\alpha\beta\zeta\rho}\omega^{(1)}_{\rho\zeta\bar{\mu}\bar{\nu}}$	$D_{\alpha\beta\bar{\mu}\bar{\nu}}(uu)$: $4(-1)^{\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+u}[u]^{-1/2}\sum_{\zeta\rho}\frac{z(0\lambda_\alpha\lambda_\beta\lambda_\rho\lambda_\zeta uu)z(0\lambda_\rho\lambda_\zeta\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}uu)}{\varepsilon_{\bar{\mu}\bar{\nu}}-\varepsilon_{\zeta\rho}}$
$\sum_{\zeta\rho} g_{\alpha\zeta\bar{\mu}\rho}\omega^{(1)}_{\rho\beta\bar{\nu}\zeta}$	$\Delta_{\alpha\beta\bar{\mu}\bar{\nu}}(UU)$: $4(-1)^{U-\lambda_{\bar{\mu}}}[U]^{1/2}\sum_{ud}\sum_{\zeta\rho}(-1)^{\lambda_\zeta+d}\frac{[u,d]^{1/2}}{\varepsilon_{\bar{\nu}\zeta}-\varepsilon_{\beta\rho}}$ $\times\begin{Bmatrix}\lambda_\alpha & \lambda_\beta & U\\ \lambda_\zeta & d & \lambda_{\bar{\nu}}\\ u & \lambda_\rho & \lambda_{\bar{\mu}}\end{Bmatrix}z(0\lambda_\alpha\lambda_\zeta\lambda_\rho\lambda_{\bar{\mu}}uu)z(0\lambda_\rho\lambda_\beta\lambda_\zeta\lambda_{\bar{\nu}}dd)$

Tab. 14: The multipliers for three- and four-particle effective matrix elements of $\widehat{\Omega}^{(2)}$

Construction	SU(2)–invariant: Expression
$v_{\alpha\bar{\mu}}\omega^{(1)}_{\beta\zeta\bar{\nu}\bar{\eta}}$	$T_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(u\tau_1)$: $2(-1)^{\lambda_{\bar{\nu}}+\lambda_{\bar{\eta}}+u}\frac{f(\tau_1\lambda_\alpha\lambda_{\bar{\mu}})}{\varepsilon_{\bar{\nu}\bar{\eta}}-\varepsilon_{\beta\zeta}}z(0\lambda_\beta\lambda_\zeta\lambda_{\bar{\eta}}\lambda_{\bar{\nu}}uu)$
$g_{\beta\zeta\bar{\nu}\bar{\eta}}\omega^{(1)}_{\alpha\bar{\mu}}$	$T'_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(u\tau_2)$: $\widehat{R}\left(\begin{smallmatrix}\bar{\nu}\bar{\eta}\to\bar{\mu}\\ \beta\zeta\to\alpha\end{smallmatrix}\right)T_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(u\tau_2)$
$\sum_{\rho} g_{\alpha\beta\bar{\mu}\rho}\omega^{(1)}_{\rho\zeta\bar{\nu}\bar{\eta}}$	$(-1)^M T_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(DdU)$: $4(-1)^{\lambda_{\bar{\eta}}-\lambda_{\bar{\nu}}+\lambda_\zeta+U}[D]^{1/2}\sum_{u\rho}\frac{(-1)^{\lambda_\rho}}{\varepsilon_{\bar{\nu}\bar{\eta}}-\varepsilon_{\zeta\rho}}[u]^{1/2}z(0\lambda_\alpha\lambda_\beta\lambda_\rho\lambda_{\bar{\mu}}uu)$ $\times z(0\lambda_\rho\lambda_\zeta\lambda_{\bar{\eta}}\lambda_{\bar{\nu}}dd)\begin{Bmatrix}D & d & U\\ \lambda_\rho & \lambda_\beta & \lambda_\zeta\end{Bmatrix}\begin{Bmatrix}\lambda_\alpha & \lambda_\beta & u\\ \lambda_\rho & \lambda_{\bar{\mu}} & U\end{Bmatrix}$
$g_{\alpha\beta\bar{\mu}\bar{\nu}}\omega^{(1)}_{\zeta\rho\bar{\eta}\bar{\sigma}}$	$Q_{\alpha\beta\zeta\rho\bar{\mu}\bar{\nu}\bar{\eta}\bar{\sigma}}(ud)$: $\frac{4}{\varepsilon_{\bar{\eta}\bar{\sigma}}-\varepsilon_{\zeta\rho}}(-1)^{u+d+\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+\lambda_{\bar{\eta}}+\lambda_{\bar{\sigma}}}z(0\lambda_\alpha\lambda_\beta\lambda_{\bar{\nu}}\lambda_{\bar{\mu}}uu)z(0\lambda_\zeta\lambda_\rho\lambda_{\bar{\sigma}}\lambda_{\bar{\eta}}dd)$

$$o(\tau_i\lambda_\alpha\lambda_{\bar\beta}) \stackrel{\text{def}}{=} (-1)^{\lambda_\alpha-\lambda_{\bar\beta}}[\tau_i]^{-1}\sum_{m_i=-\tau_i}^{+\tau_i}(-1)^{m_i-e(\tau_i m_i)}, \tag{4.8}$$

which is easy to derive considering the properties of the self-adjoint operator v_i: $v_{\alpha\bar\beta}=v_{\bar\beta\alpha}$ and $v^{\tau_i\dagger}_{m_i}=(-1)^{e(\tau_i m_i)}v^{\tau_i}_{-m_i}$. The phase multiplier $e(\tau_i m_i)$ is optional. Usually, two possibilities are exploited, one that is given by $e(\tau_i m_i)=m_i$ [8, Eq. (25)], and the other by $e(\tau_i m_i)=\tau_i-m_i$ [11, Eq. (2.3)]. It is to be noticed that throughout the present text, the second possibility is preferred. In this case, $o(\tau_i\lambda_\alpha\lambda_{\bar\beta})=(-1)^{\lambda_\alpha-\lambda_{\bar\beta}+\tau_i}$.

The index i distinguishes the interaction operators v_i that befit to a second quantised form $\widehat{V}_1$: for $\widehat{V}_1$ in Eq. (4.3), $i=0$; for $\widehat{V}_1$ in Eq. (4.2), $i=1$; for $\widehat{V}_1$ in Eq. (4.1), $i=2$.

In Tabs. 12-14, the abbreviation $\varepsilon_{xy\ldots z}=\varepsilon_x+\varepsilon_y+\ldots+\varepsilon_z$, where ε_x is the single-electron energy (refer to Eq. (2.65)). The operator $\widehat{R}$ replaces orbitals in energy denominators. Thus, for example, $\widehat{R}\binom{\bar\nu\bar\eta\to\bar\mu}{\beta\zeta\to\alpha}(\varepsilon_{\bar\nu\bar\eta}-\varepsilon_{\beta\zeta})^{-1}=(\varepsilon_{\bar\mu}-\varepsilon_\alpha)^{-1}$.

The first-order effective matrix elements $\omega^{(1)}$, $\widetilde{\omega}^{(1)}$ are defined by (see Eq. (2.65))

$$\omega^{(1)}_{\alpha\bar\beta}\stackrel{\text{def}}{=}\frac{v_{\alpha\bar\beta}}{\varepsilon_{\bar\beta}-\varepsilon_\alpha},\quad \omega^{(1)}_{\alpha\beta\bar\mu\bar\nu}\stackrel{\text{def}}{=}\frac{g_{\alpha\beta\bar\mu\bar\nu}}{\varepsilon_{\bar\mu\bar\nu}-\varepsilon_{\alpha\beta}},\quad \widetilde{\omega}^{(1)}_{\alpha\beta\bar\mu\bar\nu}\stackrel{\text{def}}{=}\omega^{(1)}_{\alpha\beta\bar\mu\bar\nu}-\omega^{(1)}_{\alpha\beta\bar\nu\bar\mu}. \tag{4.9}$$

Recalling the properties of $v_{\alpha\bar\beta}$, $g_{\alpha\beta\bar\mu\bar\nu}$ (also, see Eq. (3.55)), it is easy to deduce that the matrix representations $\omega^{(1)}$, $\widetilde{\omega}^{(1)}$ satisfy $\omega^{(1)}_{\alpha\bar\beta}=-\omega^{(1)}_{\bar\beta\alpha}$ and

$$\omega^{(1)}_{\alpha\beta\bar\mu\bar\nu}=\omega^{(1)}_{\beta\alpha\bar\nu\bar\mu}=-\omega^{(1)}_{\bar\nu\bar\mu\beta\alpha}=-\omega^{(1)}_{\bar\mu\bar\nu\alpha\beta}, \tag{4.10a}$$

$$\widetilde{\omega}^{(1)}_{\alpha\beta\bar\mu\bar\nu}=\widetilde{\omega}^{(1)}_{\beta\alpha\bar\nu\bar\mu}=\widetilde{\omega}^{(1)}_{\bar\mu\bar\nu\beta\alpha}=\widetilde{\omega}^{(1)}_{\bar\nu\bar\mu\alpha\beta}$$
$$=-\widetilde{\omega}^{(1)}_{\alpha\beta\bar\nu\bar\mu}=-\widetilde{\omega}^{(1)}_{\beta\alpha\bar\mu\bar\nu}=-\widetilde{\omega}^{(1)}_{\bar\nu\bar\mu\beta\alpha}=-\widetilde{\omega}^{(1)}_{\bar\mu\bar\nu\alpha\beta}. \tag{4.10b}$$

Now, it becomes clear why it suffices to consider only 13 constructions from the large number of terms.

To distinguish the $\mathrm{SU}(2)$–invariants by the summation parameters, the following special notations are used.

μ	c	v	e
$S_{\alpha\bar\beta}(\tau_1\tau_2\tau)$	$S_{\alpha\bar\beta}(\tau_1\tau_2\tau)$	$\dot{S}_{\alpha\bar\beta}(\tau_1\tau_2\tau)$	$\ddot{S}_{\alpha\bar\beta}(\tau_1\tau_2\tau)$

(4.11)

ζ	c	c
$\bar\mu$	v	e
$\widetilde{S}_{\alpha\bar\beta}(\tau_1)$	$\widetilde{\dot{S}}_{\alpha\bar\beta}(\tau_1)$	$\widetilde{\ddot{S}}_{\alpha\bar\beta}(\tau_1)$
$\widetilde{S}'_{\alpha\bar\beta}(\tau_2)$	$\widetilde{\dot{S}}'_{\alpha\bar\beta}(\tau_2)$	$\widetilde{\ddot{S}}'_{\alpha\bar\beta}(\tau_2)$

(4.12)

ζ	c	v	e
$D_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_1)$	$D_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_1)$	$\dot{D}_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_1)$	$\ddot{D}_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_1)$
$D'_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_2)$	$D'_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_2)$	$\dot{D}'_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_2)$	$\ddot{D}'_{\alpha\beta\bar\mu\bar\nu}(Uu\tau_2)$

(4.13)

ζ	c	v	e	e	v
ρ	c	v	e	v	e
$D_{\alpha\beta\bar\mu\bar\nu}(uu)$	$D_{\alpha\beta\bar\mu\bar\nu}(uu)$	$\dot{D}_{\alpha\beta\bar\mu\bar\nu}(uu)$	$\ddot{D}_{\alpha\beta\bar\mu\bar\nu}(uu)$	$\dddot{D}_{\alpha\beta\bar\mu\bar\nu}(uu)$	$\dddot{D}_{\alpha\beta\bar\mu\bar\nu}(uu)$

(4.14)

ζ	c	c
ρ	v	e
$\Delta_{\alpha\beta\bar\mu\bar\nu}(UU)$	$\dot{\Delta}_{\alpha\beta\bar\mu\bar\nu}(UU)$	$\ddot{\Delta}_{\alpha\beta\bar\mu\bar\nu}(UU)$

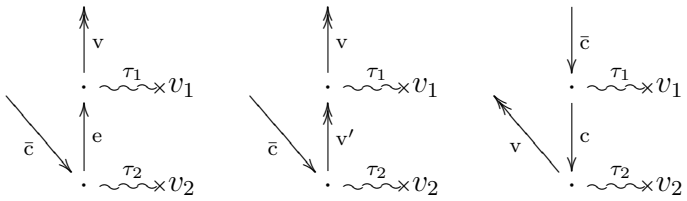
(4.15)

ρ	c	v	e
$T_{\alpha\beta\zeta\bar\mu\bar\nu\bar\eta}(DdU)$	$T_{\alpha\beta\zeta\bar\mu\bar\nu\bar\eta}(DdU)$	$\dot{T}_{\alpha\beta\zeta\bar\mu\bar\nu\bar\eta}(DdU)$	$\ddot{T}_{\alpha\beta\zeta\bar\mu\bar\nu\bar\eta}(DdU)$

(4.16)

Particularly, for $\widetilde{S}_{\alpha\bar{\beta}}$, $\zeta = \mathrm{c}$, $\eta = \mathrm{v}$, $\rho = \mathrm{e}$. To designate that the direct and exchanged parts of a two-particle matrix element are involved, the additional tildes are exploited. Thus $\widetilde{D}_{\alpha\beta\bar{\mu}\bar{\nu}}(Uu\tau_1)$ implies that the two-particle matrix representation reads $\widetilde{\omega}^{(1)}_{\zeta\beta\bar{\mu}\bar{\nu}}$. Conversely, $\widetilde{D'}_{\alpha\beta\bar{\mu}\bar{\nu}}(Uu\tau_2)$ implies that the two-particle matrix representation reads $\widetilde{g}_{\zeta\beta\bar{\mu}\bar{\nu}}$. If written $D_{\alpha\beta\bar{\mu}\bar{\nu}}(\widetilde{u}u)$ $(\Delta_{\alpha\beta\bar{\mu}\bar{\nu}}(\widetilde{U}U))$, then the considered matrix representation is $\widetilde{g}_{\alpha\beta\zeta\rho}$ $(\widetilde{g}_{\alpha\zeta\bar{\mu}\rho})$; if written $D_{\alpha\beta\bar{\mu}\bar{\nu}}(u\widetilde{u})$ $(\Delta_{\alpha\beta\bar{\mu}\bar{\nu}}(U\widetilde{U}))$, then the corresponding matrix representation is $\widetilde{\omega}^{(1)}_{\rho\zeta\bar{\mu}\bar{\nu}}$ $(\widetilde{\omega}_{\rho\beta\bar{\nu}\zeta})$; if written $\widetilde{D}_{\alpha\beta\bar{\mu}\bar{\nu}}(uu)$ $(\widetilde{\Delta}_{\alpha\beta\bar{\mu}\bar{\nu}}(UU))$, then the matrix representations g and $\omega^{(1)}$ are both with tildes. The similar arguments hold and for the rest of $\mathrm{SU}(2)$–invariants. Also, it should be noted that for each two-particle matrix representation with tilde, the corresponding z coefficient is given by Eq. (3.64).

Example. Consider the sum of three Goldstone diagrams:



where the double arrow distinguishes the valence electron states. Since $\tau_1 \neq 0$, $\tau_2 \neq 0$, these diagrams involve the interaction of atom with some external field (e.g. electric). By Lemma 2.3.9, given diagrams denote the one-body terms of $\widehat{\Omega}^{(2)}$. Their algebraic equivalent reads

$$\sum_{\mathrm{v}\bar{\mathrm{c}}}\sum_{\mathrm{e}} a_{\mathrm{v}}a^{\dagger}_{\bar{\mathrm{c}}}\,\frac{v_{\mathrm{ve}}\omega^{(1)}_{\mathrm{e}\bar{\mathrm{c}}}}{\varepsilon_{\bar{\mathrm{c}}}-\varepsilon_{\mathrm{v}}} + \sum_{\mathrm{v}\bar{\mathrm{c}}}\sum_{\mathrm{v}'} a_{\mathrm{v}}a^{\dagger}_{\bar{\mathrm{c}}}\,\frac{v_{\mathrm{vv}'}\omega^{(1)}_{\mathrm{v}'\bar{\mathrm{c}}}}{\varepsilon_{\bar{\mathrm{c}}}-\varepsilon_{\mathrm{v}}} + \sum_{\mathrm{v}\bar{\mathrm{c}}}\sum_{\mathrm{c}} a_{\mathrm{v}}a^{\dagger}_{\bar{\mathrm{c}}}\,\frac{v_{\mathrm{c}\bar{\mathrm{c}}}\omega^{(1)}_{\mathrm{vc}}}{\varepsilon_{\mathrm{v}}-\varepsilon_{\bar{\mathrm{c}}}}.$$

Now, arrange a given expression in terms of $\mathrm{SU}(2)$–invariants. By using Tab. 12 and Eq. (4.11), it follows that the first two terms are easy to obtain with $\alpha = \mathrm{v}$, $\bar{\beta} = \bar{\mathrm{c}}$ and $\mu = \mathrm{e}, \mathrm{v}'$. The corresponding $\mathrm{SU}(2)$–invariants are $\ddot{S}_{\mathrm{v}\bar{\mathrm{c}}}(\tau_1\tau_2\tau)$ (for $\mu = \mathrm{e}$) and $\dot{S}_{\mathrm{v}\bar{\mathrm{c}}}(\tau_1\tau_2\tau)$ (for $\mu = \mathrm{v}'$).

The last term (diagram) must be written in a standard form, as it does not satisfy a given construction for $S_{\alpha\bar{\beta}}(\tau_1\tau_2\tau)$. Make use of the symmetry properties of $v_{\alpha\bar{\beta}}$ and $\omega^{(1)}_{\alpha\bar{\beta}}$. Then

$$\sum_{\mathrm{v}\bar{\mathrm{c}}}\sum_{\mathrm{c}} a_{\mathrm{v}}a^{\dagger}_{\bar{\mathrm{c}}}\,\frac{v_{\mathrm{c}\bar{\mathrm{c}}}\omega^{(1)}_{\mathrm{vc}}}{\varepsilon_{\mathrm{v}}-\varepsilon_{\bar{\mathrm{c}}}} = \sum_{\mathrm{v}\bar{\mathrm{c}}}\sum_{\mathrm{c}} a_{\mathrm{v}}a^{\dagger}_{\bar{\mathrm{c}}}\,\frac{v_{\bar{\mathrm{c}}\mathrm{c}}\omega^{(1)}_{\mathrm{cv}}}{\varepsilon_{\bar{\mathrm{c}}}-\varepsilon_{\mathrm{v}}}$$

and thus the corresponding $\mathrm{SU}(2)$–invariant is $S_{\bar{\mathrm{c}}\mathrm{v}}(\tau_1\tau_2\tau)$ with $\alpha = \bar{\mathrm{c}}$, $\bar{\beta} = \mathrm{v}$, $\mu = \mathrm{c}$. Finally, the given sum of diagrams yields

$$\sum_{\mathrm{v}\bar{\mathrm{c}}}(\varepsilon_{\bar{\mathrm{c}}}-\varepsilon_{\mathrm{v}})^{-1}\sum_{\tau m}\Big(W^{\tau}_{m}(\lambda_{\mathrm{v}}\widetilde{\lambda}_{\bar{\mathrm{c}}})\big(\dot{S}_{\mathrm{v}\bar{\mathrm{c}}}(\tau_1\tau_2\tau)+\ddot{S}_{\mathrm{v}\bar{\mathrm{c}}}(\tau_1\tau_2\tau)\big)+(-1)^{\lambda_{\mathrm{v}}-\lambda_{\bar{\mathrm{c}}}+m}W^{\tau}_{-m}(\lambda_{\mathrm{v}}\widetilde{\lambda}_{\bar{\mathrm{c}}})S_{\bar{\mathrm{c}}\mathrm{v}}(\tau_1\tau_2\tau)\Big).$$

Also, it is interesting to notice that particularly for $e(\tau_i m_i) = \tau_i - m_i$ (see Eqs. (4.7)-(4.8)),

$$S_{\bar{\mathrm{c}}\mathrm{v}}(\tau_1\tau_2\tau) = (-1)^{\lambda_{\mathrm{v}}-\lambda_{\bar{\mathrm{c}}}+\tau_1+\tau_2}\widehat{R}\big(\substack{\bar{\mathrm{c}}\to\mathrm{v}\\ \mathrm{c}\to\mathrm{c}}\big)\overline{S_{\mathrm{v}\bar{\mathrm{c}}}(\tau_1\tau_2\tau)}.$$

Thus the third diagram represents some complex conjugate—the reflection about a horizontal axis—of a diagram that is characterised by the $\mathrm{SU}(2)$–invariant $S_{\mathrm{v}\bar{\mathrm{c}}}(\tau_1\tau_2\tau)$.

The example indicates that the Goldstone diagrams are represented by the two types of irreducible tensor operators: $\widehat{O}^{\Lambda}_{+M}$ and $\widehat{O}^{\Lambda}_{-M}$. The analysis of all generated terms of $\widehat{\Omega}^{(2)}$ leads to the following conclusions. The terms (diagrams) associated to the tensor structure $\widehat{O}^{\Lambda}_{-M}$ are: (i) the folded diagrams; (ii) some diagrams, obtained by contracting the core orbitals in Wick's series; (iii) the diagrams, acceded to the reflection about a horizontal axis of a number of diagrams associated to the tensor structure $\widehat{O}^{\Lambda}_{+M}$.

To distinguish the considered two types of terms, the superscripts $\pm$ over the matrix representations are used so that for $n=1,2,3,4$, the $\mathrm{SU}(2)$–invariants $\Omega^{(2)\pm}$ of each n–body part of $\widehat{\Omega}^{(2)}$ are given by

$$\omega^{(2)\pm}_{\alpha\bar{\beta}} = (-1)^{t_1^{\pm}} \sum_{\Lambda} \langle \lambda_\alpha m_\alpha \lambda_{\bar{\beta}} - m_{\bar{\beta}} | \Lambda \pm M \rangle \Omega^{(2)\pm}_{\alpha\bar{\beta}}(\Lambda), \tag{4.17a}$$

$$t_1^{+} \stackrel{\text{def}}{=} \lambda_{\bar{\beta}} + m_{\bar{\beta}}, \quad t_1^{-} \stackrel{\text{def}}{=} \lambda_\alpha + m_\alpha, \tag{4.17b}$$

$$\omega^{(2)\pm}_{\alpha\beta\bar{\mu}\bar{\nu}} = (-1)^{t_2^{\pm}} \sum_{\Lambda_1\Lambda_2\Lambda} E\begin{pmatrix} \lambda_\alpha & \lambda_\beta & \lambda_{\bar{\mu}} & \lambda_{\bar{\nu}} \\ m_\alpha & m_\beta & -m_{\bar{\mu}} & -m_{\bar{\nu}} \end{pmatrix}; \Lambda_1\Lambda_2\Lambda \pm M \Big) \Omega^{(2)\pm}_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda), \tag{4.18a}$$

$$t_2^{+} \stackrel{\text{def}}{=} \lambda_{\bar{\mu}} + \lambda_{\bar{\nu}} + m_{\bar{\mu}} + m_{\bar{\nu}}, \quad t_2^{-} \stackrel{\text{def}}{=} \lambda_\alpha + \lambda_\beta + m_\alpha + m_\beta, \tag{4.18b}$$

$$\omega^{(2)\pm}_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}} = (-1)^{t_3^{\pm}} \sum_{\Lambda_1\Lambda_2} \sum_{\Lambda_3\Lambda} (-1)^{M} \langle \lambda_\alpha m_\alpha \lambda_{\bar{\mu}} - m_{\bar{\mu}} | \Lambda_3 \pm M_3 \rangle \Omega^{(2)\pm}_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)$$

$$\times E\begin{pmatrix} \lambda_\beta & \lambda_\zeta & \lambda_{\bar{\nu}} & \lambda_{\bar{\eta}} \\ m_\beta & m_\zeta & -m_{\bar{\nu}} & -m_{\bar{\eta}} \end{pmatrix}; \Lambda_1\Lambda_2\Lambda \mp M \Big), \tag{4.19a}$$

$$t_3^{+} \stackrel{\text{def}}{=} \lambda_{\bar{\mu}} + \lambda_{\bar{\nu}} + \lambda_{\bar{\eta}} + m_{\bar{\mu}} + m_{\bar{\nu}} + m_{\bar{\eta}}, \quad t_3^{-} \stackrel{\text{def}}{=} \lambda_\alpha + \lambda_\beta + \lambda_\zeta + m_\alpha + m_\beta + m_\zeta, \tag{4.19b}$$

$$\omega^{(2)}_{\alpha\beta\zeta\rho\bar{\mu}\bar{\nu}\bar{\eta}\bar{\sigma}} = (-1)^{t_4} \sum_{\substack{\Lambda_1\Lambda_2 \\ \Lambda_3\Lambda_4\Lambda}} (-1)^{M} \Omega^{(2)}_{\alpha\beta\zeta\rho\bar{\mu}\bar{\nu}\bar{\eta}\bar{\sigma}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)$$

$$\times E\begin{pmatrix} \lambda_\alpha & \lambda_\beta & \lambda_{\bar{\mu}} & \lambda_{\bar{\nu}} \\ m_\alpha & m_\beta & -m_{\bar{\mu}} & -m_{\bar{\nu}} \end{pmatrix}; \Lambda_1\Lambda_2\Lambda M \Big) E\begin{pmatrix} \lambda_\zeta & \lambda_\rho & \lambda_{\bar{\eta}} & \lambda_{\bar{\sigma}} \\ m_\zeta & m_\rho & -m_{\bar{\eta}} & -m_{\bar{\sigma}} \end{pmatrix}; \Lambda_3\Lambda_4\Lambda - M \Big), \tag{4.20a}$$

$$t_4 \stackrel{\text{def}}{=} \lambda_{\bar{\mu}} + \lambda_{\bar{\nu}} + \lambda_{\bar{\eta}} + \lambda_{\bar{\sigma}} + m_{\bar{\mu}} + m_{\bar{\nu}} + m_{\bar{\eta}} + m_{\bar{\sigma}} \tag{4.20b}$$

and $\omega^{(2)} = \omega^{(2)+} + \omega^{(2)-}$. The coefficients $\Omega^{(2)\pm}$ are displayed in Appendix C.

4.1.1 Remark. In Tab. 12-14, the $\mathrm{SU}(2)$–invariants are also obtained by given Eqs. (4.17)-(4.20) for the effective matrix elements with the plus sign, the basis indices $+M$, $+M_3$ and eliminated phase multiplier $(-1)^M$.

Eqs. (4.17)-(4.20) direct attention to the convenience of z-scheme to compare with b-scheme, though both of them are equivalent. The attraction is due to the coefficients E and their symmetry properties in Eq. (3.60). Conversely, for b-scheme, the associated coefficient reads $E' \equiv \widehat{\pi}_{23} E$, and thus it does not satisfy the same properties as that of E. For instance, the relationship between $\widehat{\pi}_{24} E'$ and E' is realised by

$$E\begin{pmatrix} \lambda_\alpha & \lambda_{\bar{\nu}} & \lambda_\beta & \lambda_{\bar{\mu}} \\ m_\alpha & -m_{\bar{\nu}} & m_\beta & -m_{\bar{\mu}} \end{pmatrix}; \Lambda_1\Lambda_2\Lambda M \Big) = \sum_{\overline{\Lambda}_1\overline{\Lambda}_2} (-1)^{\overline{\Lambda}_2+1} a(\lambda_{\bar{\mu}}\lambda_{\bar{\nu}}\Lambda_2)[\Lambda_1,\Lambda_2,\overline{\Lambda}_1,\overline{\Lambda}_2]^{1/2}$$

$$\times \begin{Bmatrix} \lambda_\alpha & \lambda_{\bar{\nu}} & \Lambda_1 \\ \lambda_{\bar{\mu}} & \lambda_\beta & \Lambda_2 \\ \overline{\Lambda}_1 & \overline{\Lambda}_2 & \Lambda \end{Bmatrix} E\begin{pmatrix} \lambda_\alpha & \lambda_{\bar{\mu}} & \lambda_\beta & \lambda_{\bar{\nu}} \\ m_\alpha & -m_{\bar{\mu}} & m_\beta & -m_{\bar{\nu}} \end{pmatrix}; \overline{\Lambda}_1\overline{\Lambda}_2\Lambda M \Big)$$

which implies the appearance of additional summation.

4.2 The treatment of terms of the third-order effective Hamiltonian

By Lemma 2.3.9, this part of computation requires significantly less time to compare with the handling of $\widehat{\Omega}^{(2)}$. Moreover, the non-zero terms $\widehat{h}^{(3)}_{mn;\xi}$ are derived in accordance with Theorem 2.3.12 which makes it possible to reject a large amount of terms of $\widehat{\Omega}^{(2)}$ attaching the zero-valued contributions. As already pointed out, the terms of $\widehat{\Omega}^{(2)}$ that provide non-zero contributions to $\widehat{h}^{(3)}_{mn;\xi}$, are listed in Appendix C.

In the present section, the single-particle and two-particle operators of $\widehat{\mathscr{H}^{(3)}}$ will be considered. Then (refer to Eq. (4.4)) $\widehat{O}^{\Lambda}([\lambda]\varkappa) \equiv W^{\Lambda}(\lambda_{\mathrm{v}}\widetilde{\lambda}_{\bar{\mathrm{v}}})$ is associated to the angular reduction scheme $\mathscr{T}_1^{[1^2]}$ for $m+n-\xi=1$, and $\widehat{O}^{\Lambda}([\lambda]\varkappa) \equiv -[W^{\Lambda_1}(\lambda_{\mathrm{v}}\lambda_{\mathrm{v}'}) \times W^{\Lambda_2}(\widetilde{\lambda}_{\bar{\mathrm{v}}}\widetilde{\lambda}_{\bar{\mathrm{v}}'})]^{\Lambda}$ is associated to the scheme $\mathscr{T}_1^{[2^2]}$ for $m+n-\xi=2$. Possible values of m, n, ξ are listed in Tab. 11.

Tab. 15: The expansion coefficients for one-body terms of the third-order contribution to the effective Hamiltonian

$(mn\xi)$	$\mathfrak{h}^{(3)+}_{mn;\xi}(\Lambda)$
(111)	$(-1)^{\lambda_{\rm v}-\lambda_{\bar{\rm v}}}[\tau_0]^{1/2}\sum_{\overline{\Lambda}}[\overline{\Lambda}]^{1/2}\langle\tau_0 m_0\overline{\Lambda}\,\overline{M}\vert\Lambda M\rangle\Big((-1)^{\Lambda}\sum_{\rm e} f(\tau_0\lambda_{\rm v}\lambda_{\rm e})\Omega^{(2)+}_{{\rm e}\bar{\rm v}}(\overline{\Lambda})\begin{Bmatrix}\tau_0 & \overline{\Lambda} & \Lambda\\ \lambda_{\bar{\rm v}} & \lambda_{\rm v} & \lambda_{\rm e}\end{Bmatrix}$ $-(-1)^{\overline{\Lambda}}\sum_{\rm c} f(\tau_0\lambda_{\rm c}\lambda_{\bar{\rm v}})\Omega^{(2)+}_{{\rm vc}}(\overline{\Lambda})\begin{Bmatrix}\tau_0 & \overline{\Lambda} & \Lambda\\ \lambda_{\rm v} & \lambda_{\bar{\rm v}} & \lambda_{\rm c}\end{Bmatrix}\Big)$
(212)	$2(-1)^{\lambda_{\rm v}-\lambda_{\bar{\rm v}}}\sum_{\alpha={\rm v,e}}\sum_{\rm c}(-1)^{\lambda_{\alpha'}-\lambda_{\rm c}}\sum_u \widetilde{z}(0\lambda_{\rm c}\lambda_{\rm v}\lambda_{\bar{\rm v}}\lambda_{\alpha'}uu)\Omega^{(2)+}_{\alpha'{\rm c}}(\Lambda)[u]^{1/2}\begin{Bmatrix}\Lambda & \lambda_{\alpha'} & \lambda_{\rm c}\\ u & \lambda_{\rm v} & \lambda_{\bar{\rm v}}\end{Bmatrix}$
(122)	$(-1)^{\Lambda}[\tau_0]^{1/2}\sum_{\Lambda_1\Lambda_2\overline{\Lambda}}(-1)^{\overline{\Lambda}}[\Lambda_1,\Lambda_2,\overline{\Lambda}]^{1/2}\langle\tau_0 m_0\overline{\Lambda}\,\overline{M}\vert\Lambda M\rangle\sum_{\rm c}\Big(\sum_{\rm v'}(-1)^{\lambda_{\rm c}-\lambda_{\rm v'}} f(\tau_0\lambda_{\rm c}\lambda_{\rm v'})$ $\times\widetilde{\Omega}^{(2)+}_{{\rm v'vc\bar{v}}}(\Lambda_1\Lambda_2\overline{\Lambda})\begin{Bmatrix}\lambda_{\rm v'} & \lambda_{\rm v} & \Lambda_1\\ \lambda_{\rm c} & \lambda_{\bar{\rm v}} & \Lambda_2\\ \tau_0 & \Lambda & \overline{\Lambda}\end{Bmatrix} - \sum_{\rm e} a(\lambda_{\rm e}\lambda_{\bar{\rm v}}\Lambda_2) f(\tau_0\lambda_{\rm c}\lambda_{\rm e})\Omega^{(2)+}_{{\rm ev\bar{v}c}}(\Lambda_1\Lambda_2\overline{\Lambda})\begin{Bmatrix}\lambda_{\rm e} & \lambda_{\rm v} & \Lambda_1\\ \lambda_{\rm c} & \lambda_{\bar{\rm v}} & \Lambda_2\\ \tau_0 & \Lambda & \overline{\Lambda}\end{Bmatrix}\Big)$
(223)	$2\sum_{\Lambda_1\Lambda_2}[\Lambda_1]^{1/2}\sum_{\rm cc'}\Big(a(\lambda_{\rm v}\lambda_{\bar{\rm v}}\Lambda)\sum_{\rm v'}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\rm v'}\lambda_{\bar{\rm v}}\Lambda_2\Lambda_2)\widetilde{\Omega}^{(2)+}_{{\rm vv'cc'}}(\Lambda_1\Lambda_2\Lambda)\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \lambda_{\bar{\rm v}} & \lambda_{\rm v} & \lambda_{\rm v'}\end{Bmatrix}$ $-a(\Lambda_1\Lambda_2\Lambda)\sum_{\rm e}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\bar{\rm v}}\lambda_{\rm e}\Lambda_2\Lambda_2)\Omega^{(2)+}_{{\rm evcc'}}(\Lambda_1\Lambda_2\Lambda)\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \lambda_{\bar{\rm v}} & \lambda_{\rm v} & \lambda_{\rm e}\end{Bmatrix}\Big) + 2\sum_{\Lambda_1\Lambda_2}(-1)^{\Lambda_1}[\Lambda_2]^{1/2}$ $\times\sum_{\rm c}\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \lambda_{\bar{\rm v}} & \lambda_{\rm v} & \lambda_{\rm c}\end{Bmatrix}\Big(a(\lambda_{\rm v}\lambda_{\bar{\rm v}}\Lambda)\sum_{\mu={\rm v,e}}(-1)^{\lambda_{\mu'}+\lambda_{\mu''}}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm c}\lambda_{\mu''}\lambda_{\mu'}\Lambda_1\Lambda_1)\Omega^{(2)+}_{\mu'\mu''{\rm c}\bar{\rm v}}(\Lambda_1\Lambda_2\Lambda)$ $-a(\Lambda_1\Lambda_2\Lambda)\sum_{\rm ev'}(-1)^{\lambda_{\rm e}+\lambda_{\rm v'}}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm v}\lambda_{\rm v'}\lambda_{\rm e}\Lambda_1\Lambda_1)\Omega^{(2)+}_{{\rm ev'\bar{v}c}}(\Lambda_1\Lambda_2\Lambda)\Big)$
(234)	$2\sum_{\rm cc'}\sum_{\mu={\rm v,e}}\sum_{\Lambda_2} a(\lambda_{\rm c}\lambda_{\rm c'}\Lambda_2)\Big(\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\rm v''}\lambda_{\mu'}\Lambda_2\Lambda_2)\Omega^{(2)+}_{{\rm vv''}\mu'\bar{\rm v}{\rm c'c}}(\Lambda_2\Lambda_2\Lambda 0)$ $+\sum_{\Lambda_1\Lambda_3\overline{\Lambda}}(-1)^{\lambda_{\bar{\rm v}}+\Lambda_3+\overline{M}}[\Lambda_1,\Lambda_3,\overline{\Lambda}]^{1/2}\langle\Lambda_3 M_3\overline{\Lambda}\,\overline{M}\vert\Lambda M\rangle\big((-1)^{\lambda_{\rm v''}}$ $\times\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\mu'}\lambda_{\rm v''}\Lambda_2\Lambda_2)\Omega^{(2)+}_{{\rm v''v}\mu'\bar{\rm v}{\rm c'c}}(\Lambda_1\Lambda_2\Lambda_3\overline{\Lambda})\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \overline{\Lambda}\\ \lambda_{\rm v''} & \lambda_{\rm v} & \lambda_{\mu'}\end{Bmatrix}\begin{Bmatrix}\Lambda_3 & \overline{\Lambda} & \Lambda\\ \lambda_{\rm v} & \lambda_{\bar{\rm v}} & \lambda_{\rm v''}\end{Bmatrix} + a(\Lambda_1\Lambda_2\lambda_{\rm v})$ $\times\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\mu''}\lambda_{\mu'}\Lambda_2\Lambda_2)\Omega^{(2)+}_{\mu''\mu'\rm v\bar{v}c'c}(\Lambda_1\Lambda_2\Lambda_3\overline{\Lambda})\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \lambda_{\mu''} & \lambda_{\rm v} & \lambda_{\mu'}\end{Bmatrix}\begin{Bmatrix}\Lambda_3 & \overline{\Lambda} & \Lambda\\ \lambda_{\rm v} & \lambda_{\bar{\rm v}} & \lambda_{\mu''}\end{Bmatrix}\big)\Big)$

Tab. 16: The expansion coefficients for two-body terms of the third-order contribution to the effective Hamiltonian

$(mn\xi)$	$\mathfrak{h}^{(3)+}_{mn;\xi}(\Lambda_1\Lambda_2\Lambda)$ [a]
(121)	$-[\tau_0]^{1/2}\sum_{\overline{\Lambda}_1\overline{\Lambda}}[\overline{\Lambda}_1,\overline{\Lambda}]^{1/2}\Big((-1)^{\overline{\Lambda}_1}a(\lambda_{\rm v}\lambda_{\rm v'}\tau_0)a(\Lambda_1\Lambda_2\Lambda)[\Lambda_1]^{1/2}\langle\tau_0 m_0\overline{\Lambda}\,\overline{M}\vert\Lambda M\rangle\begin{Bmatrix}\tau_0 & \Lambda_1 & \overline{\Lambda}_1\\ \Lambda_2 & \overline{\Lambda} & \Lambda\end{Bmatrix}$ $\times\sum_{\rm e} f(\tau_0\lambda_{\rm v}\lambda_{\rm e})\Omega^{(2)+}_{{\rm ev'\bar{v}\bar{v}'}}(\overline{\Lambda}_1\Lambda_2\overline{\Lambda})\begin{Bmatrix}\tau_0 & \lambda_{\rm v} & \lambda_{\rm e}\\ \lambda_{\rm v'} & \overline{\Lambda}_1 & \Lambda_1\end{Bmatrix} + (-1)^{m_0}a(\Lambda_1\Lambda_2\overline{\Lambda})[\Lambda_2]^{1/2}\langle\tau_0 - m_0\overline{\Lambda}\,\overline{M}\vert\Lambda M\rangle$ $\times\begin{Bmatrix}\tau_0 & \Lambda_2 & \overline{\Lambda}_1\\ \Lambda_1 & \overline{\Lambda} & \Lambda\end{Bmatrix}\sum_{\rm c} f(\tau_0\lambda_{\rm c}\lambda_{\bar{\rm v}'})\Omega^{(2)+}_{{\rm vv'c\bar{v}}}(\Lambda_1\overline{\Lambda}_1\overline{\Lambda})\begin{Bmatrix}\tau_0 & \lambda_{\bar{\rm v}'} & \lambda_{\rm c}\\ \lambda_{\bar{\rm v}} & \overline{\Lambda}_1 & \Lambda_2\end{Bmatrix}\Big)$
(211)	$(-1)^{\lambda_{\bar{\rm v}'}+\Lambda}\Big([\Lambda_2]^{1/2}\sum_{\rm e}(-1)^{\lambda_{\rm e}}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm v'}\lambda_{\rm e}\lambda_{\bar{\rm v}}\Lambda_1\Lambda_1)\Omega^{(2)+}_{{\rm e}\bar{\rm v}'}(\Lambda)\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \lambda_{\bar{\rm v}'} & \lambda_{\rm e} & \lambda_{\bar{\rm v}}\end{Bmatrix} - (-1)^{\lambda_{\bar{\rm v}}+\Lambda_1}[\Lambda_1]^{1/2}$ $\times\sum_{\rm c}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm v}\lambda_{\bar{\rm v}'}\lambda_{\bar{\rm v}}\Lambda_2\Lambda_2)\Omega^{(2)+}_{{\rm v'c}}(\Lambda)\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \lambda_{\rm c} & \lambda_{\rm v'} & \lambda_{\rm v}\end{Bmatrix}\Big)$
(222)	$a(\lambda_{\bar{\rm v}}\lambda_{\bar{\rm v}'}\Lambda_2)[\Lambda_2]^{-1/2}\sum_{\rm cc'}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\bar{\rm v}'}\lambda_{\bar{\rm v}}\Lambda_2\Lambda_2)\Omega^{(2)+}_{{\rm vv'cc'}}(\Lambda_1\Lambda_2\Lambda) + [\Lambda_1]^{-1/2}$ $\times\sum_{\rm e}\sum_{\mu={\rm v,e}}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm v'}\lambda_{\mu''}\lambda_{\rm e}\Lambda_1\Lambda_1)\Omega^{(2)+}_{{\rm e}\mu''\bar{\rm v}\bar{\rm v}'}(\Lambda_1\Lambda_2\Lambda) + 2(-1)^{\Lambda_1+\Lambda_2}[\Lambda_1,\Lambda_2]^{1/2}\sum_{\overline{\Lambda}_1\overline{\Lambda}_2 u}[\overline{\Lambda}_1]^{1/2}$ $\times[\overline{\Lambda}_2,u]^{1/2}\sum_{\rm c}\Big((-1)^{\overline{\Lambda}_1+\overline{\Lambda}_2}\sum_{\rm e}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm c}\lambda_{\rm e}\lambda_{\bar{\rm v}'}uu)\Omega^{(2)+}_{{\rm ev'\bar{v}c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda)\begin{Bmatrix}\lambda_{\bar{\rm v}'} & \lambda_{\rm e} & \overline{\Lambda}_1 & \overline{\Lambda}_2\\ u & \lambda_{\rm v'} & \Lambda & \lambda_{\bar{\rm v}}\\ \lambda_{\rm c} & \lambda_{\rm v} & \Lambda_1 & \Lambda_2\end{Bmatrix}$ $+(-1)^{\lambda_{\rm v'}+\lambda_{\bar{\rm v}}}\sum_{\rm v''}(-1)^{\lambda_{\rm c}+\lambda_{\rm v''}}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm c}\lambda_{\rm v''}\lambda_{\bar{\rm v}'}uu)\widetilde{\Omega}^{(2)+}_{{\rm v'v''c\bar{v}}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda)\begin{Bmatrix}\lambda_{\bar{\rm v}'} & \lambda_{\rm v''} & \overline{\Lambda}_1 & \overline{\Lambda}_2\\ u & \lambda_{\rm v'} & \Lambda & \lambda_{\bar{\rm v}}\\ \lambda_{\rm c} & \lambda_{\rm v} & \Lambda_1 & \Lambda_2\end{Bmatrix}\Big)$
(132)	$(-1)^{\tau_0+M}[\tau_0,\Lambda_2,\Lambda]^{1/2}\sum_{\rm c}\sum_{\mu={\rm v,e}}\sum_{\overline{\Lambda}_2\Lambda_3\overline{\Lambda}\vartheta}(-1)^{\overline{\Lambda}}[\overline{\Lambda}_2,\Lambda_3,\vartheta]^{1/2}\langle\Lambda_3 M_3\vartheta\varrho\vert\overline{\Lambda}\,\overline{M}\rangle$ $\times\langle\tau_0 m_0\Lambda - M\vert\vartheta\varrho\rangle\Big((-1)^{\lambda_{\rm c}-\lambda_{\mu''}+\Lambda}[\Lambda_1]^{1/2}\sum_{\overline{\Lambda}_1}[\overline{\Lambda}_1]^{1/2} f(\tau_0\lambda_{\rm c}\lambda_{\mu''})$ $\times\begin{Bmatrix}\lambda_{\bar{\rm v}} & \overline{\Lambda}_2 & \Lambda_3 & \overline{\Lambda} & \lambda_{\rm v} & \overline{\Lambda}_1\\ \lambda_{\bar{\rm v}'} & \vartheta & \lambda_{\rm v'} & \lambda_{\mu''}\\ \Lambda_2 & \lambda_{\rm c} & \Lambda & \tau_0 & \Lambda_1\end{Bmatrix}\big(\Omega^{(2)+}_{{\rm vv'}\mu''\bar{\rm v}\bar{\rm v}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda}) - \delta_{\mu\rm v}a(\lambda_{\rm v'}\lambda_{\rm v''}\Lambda_1)$ $\times\Omega^{(2)+}_{{\rm vv''v'}\bar{\rm v}\bar{\rm v}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})\big) + (-1)^{\lambda_{\bar{\rm v}'}+\lambda_{\rm v''}+\Lambda_2+\Lambda_3+\vartheta}\delta_{\mu\rm v} f(\tau_0\lambda_{\rm c}\lambda_{\rm v''})\Omega^{(2)+}_{{\rm v''vv'}\bar{\rm v}\bar{\rm v}'{\rm c}}(\Lambda_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})$ $\times\begin{Bmatrix}\lambda_{\rm c} & \overline{\Lambda}_2 & \overline{\Lambda} & \Lambda_3\\ \lambda_{\bar{\rm v}'} & \Lambda_1 & \vartheta & \lambda_{\rm v''}\\ \lambda_{\bar{\rm v}} & \Lambda_2 & \Lambda & \tau_0\end{Bmatrix}\Big)$

[a] The $12j$–symbol of the first kind is given in Ref. [12, Sec. 4-33, p. 207, Eq. (33.17)]

Tab. 17: The expansion coefficients for two-body terms of the third-order contribution to the effective Hamiltonian (continued)

$(mn\xi)$	$\mathfrak{h}^{(3)+}_{mn;\xi}(\Lambda_1\Lambda_2\Lambda)$
(233)	$2[\Lambda_2]^{1/2}\sum_{\rm c}(-1)^{\lambda_{\rm c}}\sum_{\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda}}(-1)^{\overline{M}}[\Lambda_3,\overline{\Lambda}]^{1/2}\Big((-1)^{\overline{\Lambda}}\langle\Lambda_3M_3\overline{\Lambda}-\overline{M}\vert\Lambda M\rangle\big[\sum_{\rm c'}([\Lambda_1,\overline{\Lambda}_1]^{1/2}$ $\times(-1)^{\lambda_{\rm c'}+\overline{\Lambda}_1}\sum_{\mu={\rm v,e}}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\bar{\rm v}'}\lambda_{\mu''}\overline{\Lambda}_2\overline{\Lambda}_2)\{\delta_{\mu{\rm v}}\Omega^{(2)+}_{{\rm v}\mu''{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})-a(\lambda_{\rm v'}\lambda_{\mu''}\overline{\Lambda}_1)$ $\times\Omega^{(2)+}_{{\rm vv}'\mu''\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})\}\begin{Bmatrix}\overline{\Lambda}_1 & \overline{\Lambda}_2 & \overline{\Lambda}\\ \lambda_{\bar{\rm v}'} & \lambda_{\rm v'} & \lambda_{\mu''}\end{Bmatrix}\begin{Bmatrix}\lambda_{\rm v} & \lambda_{\rm v'} & \Lambda_1\\ \lambda_{\bar{\rm v}} & \lambda_{\bar{\rm v}'} & \Lambda_2\\ \Lambda_3 & \overline{\Lambda} & \Lambda\end{Bmatrix}-\delta_{\Lambda_1\overline{\Lambda}_1}(-1)^{\lambda_{\rm c'}+\Lambda_1}$ $\times\sum_{\rm v''}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\bar{\rm v}'}\lambda_{\rm v''}\overline{\Lambda}_2\overline{\Lambda}_2)\Omega^{(2)+}_{{\rm v}''{\rm vv}'\bar{\rm v}{\rm c}'{\rm c}}(\Lambda_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})\begin{Bmatrix}\Lambda_2 & \overline{\Lambda}_2 & \Lambda_3\\ \lambda_{\rm v''} & \lambda_{\bar{\rm v}} & \lambda_{\bar{\rm v}'}\end{Bmatrix}\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \Lambda_3 & \overline{\Lambda} & \overline{\Lambda}_2\end{Bmatrix}\big)-(-1)^{\lambda_{\rm v'}+\Lambda_1}$ $\times[\Lambda_1,\overline{\Lambda}_2]^{1/2}\sum_{\rm v''}\sum_{\mu={\rm v,e}}(-1)^{\lambda_{\rm v''}+\lambda_{\bar{\mu}''}+\overline{\Lambda}_1+\overline{\Lambda}_2}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm c}\lambda_{\bar{\mu}''}\lambda_{\rm v''}\overline{\Lambda}_1\overline{\Lambda}_1)\Omega^{(2)+}_{{\rm v}'{\rm v}''\bar{\mu}''\bar{\rm v}\bar{\rm v}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})$ $\times\begin{Bmatrix}\overline{\Lambda}_1 & \overline{\Lambda}_2 & \overline{\Lambda}\\ \lambda_{\bar{\rm v}'} & \lambda_{\rm v} & \lambda_{\rm c}\end{Bmatrix}\begin{Bmatrix}\lambda_{\rm v'} & \lambda_{\rm v} & \Lambda_1\\ \lambda_{\bar{\rm v}} & \lambda_{\bar{\rm v}'} & \Lambda_2\\ \Lambda_3 & \overline{\Lambda} & \Lambda\end{Bmatrix}\big]+(-1)^{\lambda_{\bar{\rm v}}+\Lambda_2+\Lambda_3+\Lambda}[\Lambda_1,\overline{\Lambda}_1,\overline{\Lambda}_2]^{1/2}\langle\Lambda_3M_3\overline{\Lambda}\,\overline{M}\vert\Lambda M\rangle\sum_u[u]^{1/2}$ $\times\big[(-1)^{\overline{\Lambda}_1}\sum_{\mu={\rm v,e}}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm c}\lambda_{\bar{\mu}''}\lambda_{\mu''}uu)\Omega^{(2)+}_{\mu''\bar{\mu}''{\rm v}'\bar{\rm v}\bar{\rm v}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})\begin{Bmatrix}u & & \lambda_{\bar{\rm v}} & \lambda_{\rm c} & & \lambda_{\bar{\rm v}'} & \lambda_{\rm v} & & \Lambda_2\\ & \lambda_{\mu''} & & & \overline{\Lambda}_2 & & & \Lambda_1 & \\ \lambda_{\bar{\mu}''} & & \Lambda_3 & \overline{\Lambda}_1 & & \overline{\Lambda} & \lambda_{\rm v'} & & \Lambda\end{Bmatrix}$ $+(-1)^{\lambda_{\rm v'}}\sum_{\rm v''}\Big(\sum_{\rm e}(-1)^{\lambda_{\rm e}}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm c}\lambda_{\rm e}\lambda_{\rm v''}uu)\Omega^{(2)+}_{{\rm v}''{\rm v}'{\rm e}\bar{\rm v}\bar{\rm v}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})$ $\times\begin{Bmatrix}u & & \lambda_{\bar{\rm v}} & \lambda_{\rm c} & & \lambda_{\bar{\rm v}'} & \lambda_{\rm v} & & \Lambda_2\\ & \lambda_{\rm v''} & & & \overline{\Lambda}_2 & & & \Lambda_1 & \\ \lambda_{\rm e} & & \Lambda_3 & \overline{\Lambda}_1 & & \overline{\Lambda} & \lambda_{\rm v'} & & \Lambda\end{Bmatrix}-(-1)^{\Lambda_1+u}\sum_{\bar{\rm v}''}(-1)^{\lambda_{\bar{\rm v}''}}\widetilde{z}(0\lambda_{\rm v}\lambda_{\rm c}\lambda_{\bar{\rm v}''}\lambda_{\rm v''}uu)$ $\times\Omega^{(2)+}_{\bar{\rm v}''{\rm v}'{\rm v}''\bar{\rm v}\bar{\rm v}'{\rm c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_3\overline{\Lambda})\begin{Bmatrix}u & & \lambda_{\bar{\rm v}} & \lambda_{\rm c} & & \lambda_{\bar{\rm v}'} & \lambda_{\rm v} & & \Lambda_2\\ & \lambda_{\bar{\rm v}''} & & & \overline{\Lambda}_2 & & & \Lambda_1 & \\ \lambda_{\rm v''} & & \Lambda_3 & \overline{\Lambda}_1 & & \overline{\Lambda} & \lambda_{\rm v'} & & \Lambda\end{Bmatrix}\big)\big]\Big)$
(244)	$2\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda 0}(-1)^{\lambda_{\bar{\rm v}}+\lambda_{\bar{\rm v}'}}\sum_{\rm cc'\overline{\Lambda}_2}\Big(\sum_{\rm v''}\big(\sum_{\bar{\rm v}''}a(\lambda_{\rm v''}\lambda_{\bar{\rm v}''}\Lambda_1)\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\bar{\rm v}''}\lambda_{\rm v''}\overline{\Lambda}_2\overline{\Lambda}_2)$ $\times\Omega^{(2)}_{{\rm vv}'{\rm v}''\bar{\rm v}''\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\Lambda_1\Lambda_1\overline{\Lambda}_2\overline{\Lambda}_20)+\sum_{\rm e\overline{\Lambda}}[\overline{\Lambda}]\big[a(\lambda_{\rm e}\lambda_{\rm v''}\overline{\Lambda}_2)[\Lambda_1,\overline{\Lambda}_2]^{-1/2}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\rm v''}\lambda_{\rm e}\overline{\Lambda}_2\overline{\Lambda}_2)$ $\times\Omega^{(2)}_{{\rm ev}''{\rm vv}'\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_1\overline{\Lambda}_2\overline{\Lambda})-\sum_{\Lambda_3\Lambda_4}[\overline{\Lambda}_2,\Lambda_3]^{1/2}(-1)^{\Lambda_4}a(\lambda_{\rm e}\lambda_{\rm v'}\Lambda_1)\begin{Bmatrix}\Lambda_1 & \overline{\Lambda}_2 & \overline{\Lambda}\\ \lambda_{\rm e} & \lambda_{\rm v'} & \lambda_{\rm v}\end{Bmatrix}\begin{Bmatrix}\Lambda_3 & \Lambda_4 & \overline{\Lambda}\\ \lambda_{\rm e} & \lambda_{\rm v'} & \lambda_{\rm v''}\end{Bmatrix}$ $\times\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\rm v''}\lambda_{\rm e}\Lambda_4\Lambda_4)\{\Omega^{(2)}_{{\rm evv}'{\rm v}''\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_3\Lambda_4\overline{\Lambda})-a(\lambda_{\rm v'}\lambda_{\rm v''}\Lambda_3)\Omega^{(2)}_{{\rm evv}''{\rm v}'\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_3\Lambda_4\overline{\Lambda})\}\big]\big)$ $+\sum_{\mu={\rm v,e}}\sum_{\overline{\Lambda}}[\overline{\Lambda}][\Lambda_1,\overline{\Lambda}_2]^{-1/2}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\bar{\mu}''}\lambda_{\mu''}\overline{\Lambda}_2\overline{\Lambda}_2)\Omega^{(2)}_{\mu''\bar{\mu}''{\rm vv}'\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_1\overline{\Lambda}_2\overline{\Lambda})$ $+\sum_{\rm v''\bar{\rm v}''}\sum_{\Lambda_3\Lambda_4\overline{\Lambda}}a(\Lambda_1\Lambda_3\lambda_{\bar{\rm v}''})[\overline{\Lambda}][\overline{\Lambda}_2,\Lambda_3]^{1/2}\widetilde{z}(0\lambda_{\rm c}\lambda_{\rm c'}\lambda_{\bar{\rm v}''}\lambda_{\rm v''}\Lambda_4\Lambda_4)\begin{Bmatrix}\Lambda_1 & \overline{\Lambda}_2 & \overline{\Lambda}\\ \lambda_{\bar{\rm v}''} & \lambda_{\rm v'} & \lambda_{\rm v}\end{Bmatrix}\begin{Bmatrix}\Lambda_3 & \Lambda_4 & \overline{\Lambda}\\ \lambda_{\bar{\rm v}''} & \lambda_{\rm v'} & \lambda_{\rm v''}\end{Bmatrix}$ $\times[\Omega^{(2)}_{\bar{\rm v}''{\rm vv}''{\rm v}'\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_3\Lambda_4\overline{\Lambda})+a(\lambda_{\rm v}\lambda_{\rm v'}\overline{\Lambda}_2)a(\lambda_{\rm v''}\lambda_{\bar{\rm v}''}\Lambda_3)\Omega^{(2)}_{{\rm v}\bar{\rm v}''{\rm v}'{\rm v}''\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_3\Lambda_4\overline{\Lambda})$ $-a(\Lambda_3\Lambda_4\lambda_{\rm v'})\{\Omega^{(2)}_{\bar{\rm v}''{\rm vv}''{\rm v}'\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_3\Lambda_4\overline{\Lambda})+(-1)^{\lambda_{\rm v''}+\Lambda_3}a(\lambda_{\rm v}\lambda_{\rm v'}\overline{\Lambda}_2)$ $\times\Omega^{(2)}_{{\rm v}\bar{\rm v}''{\rm v}''{\rm v}'\bar{\rm v}'\bar{\rm v}{\rm c}'{\rm c}}(\overline{\Lambda}_2\Lambda_1\Lambda_3\Lambda_4\overline{\Lambda})\}\big]\Big)$

The expansion coefficients $\mathfrak{h}^{(3)}_{mn;\xi}$ associated to the irreducible tensor operator $\widehat{O}^{\Lambda}$ are given by the sum of $\mathfrak{h}^{(3)+}_{mn;\xi}$ and $\mathfrak{h}^{(3)-}_{mn;\xi}$. The sign of $\mathfrak{h}^{(3)\pm}_{mn;\xi}$ is related to the sign of $\widehat{\Omega}^{(2)\pm}$. Particularly, the coefficients $\mathfrak{h}^{(3)+}_{mn;\xi}$ are found in Tabs. 15-17. The coefficients $\mathfrak{h}^{(3)-}_{mn;\xi}$ are derived from $\mathfrak{h}^{(3)+}_{mn;\xi}$ by making the following alterations:

(a) $\Omega^{(2)+}_{\alpha\bar{\beta}}(\Lambda)\rightarrow(-1)^{\lambda_\alpha+\lambda_{\bar{\beta}}+M+1}\Omega^{(2)-}_{\alpha\bar{\beta}}(\Lambda)$

(b) $\Omega^{(2)+}_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda)\rightarrow(-1)^{\lambda_\alpha+\lambda_\beta+\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+M}\Omega^{(2)-}_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda)$

(c) $\Omega^{(2)+}_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)\rightarrow(-1)^{\lambda_\alpha+\lambda_\beta+\lambda_\zeta+\lambda_{\bar{\mu}}+\lambda_{\bar{\nu}}+\lambda_{\bar{\eta}}+M+M_3+1}\Omega^{(2)-}_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)$

In addition, there holds one more rule: (d) each basis index drawn in $\mathfrak{h}^{(3)+}_{mn;\xi}$ is replaced by the opposite sign index except for m_0. In tables, the quantities $\widetilde{\Omega}^{(2)\pm}$ satisfy

$$\widetilde{\Omega}^{(2)\pm}_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda)=\Omega^{(2)\pm}_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda)-a(\lambda_\alpha\lambda_\beta\Lambda_1)\Omega^{(2)\pm}_{\beta\alpha\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda). \tag{4.21}$$

It is now easy to bring to a decision the applicability of terms of $\widehat{\mathscr{H}}^{(3)}$ given by Eq. (4.4).

1. The third-order contributions to the effective Hamiltonian $\widehat{\mathscr{H}}^{(3)}$ are written in an operator form providing an opportunity to construct their matrix representations efficiently

– the task is confined to the calculation of matrix elements of irreducible tensor operators that are written apart from the projection-independent parts. These particular angular coefficients contain $\Omega^{(2)\pm}$ multiplied by the $3nj$–symbols.

2. The determination of $\mathrm{SU}(2)$–invariants of $\widehat{\Omega}^{(2)}$ makes it possible to settle down a number of terms (Goldstone diagrams) associated to the sole tensor structure. As a result, the latter approach permits to ascertain the contribution of n–particle ($n = 1, 2, 3, 4$) effects in CC approximation. This is done by simply replacing $\Omega^{(2)\pm}$ with Ω_n found from Eqs. (4.17)-(4.20). In this case, replace the corresponding effective matrix element $\omega^{(2)}$ with ω, where ω denotes the valence singles, doubles, triples and quadruples amplitude.

3. The terms of $\widehat{\mathscr{H}}^{(3)}$ account for the interaction of atom with external field. This is drawn in the matrix representations of v_i that represents the electric, magnetic, hyperfine, etc. interaction operator.

4. The terms of $\widehat{\mathscr{H}}^{(3)}$ are applicable to the study of both nonrelativistic and relativistic approximations. These effects are embodied in z coefficients.

4.3 Concluding remarks and discussion

In Sec. 4, an algebraic technique to evaluate the terms of MBPT has been suggested. The method relies on Lemma 2.3.9 and Theorem 2.3.12. The advantage of method reveals itself especially in the higher-order MBPT, when a huge number of terms is generated.

The restriction of space $\mathcal{H}$ the operator $\widehat{\Omega}^{(2)}$ acts on to its $\mathrm{SU}(2)$–irreducible subspaces $\mathcal{H}^{\Lambda}$ makes it possible to find the 13 non-equivalent $\mathrm{SU}(2)$–invariants, as demonstrated in Tabs. 12-14. Due to the symmetry properties of matrix representations $v_{\alpha\bar{\beta}}$, $g_{\alpha\beta\bar{\mu}\bar{\nu}}$, these invariants are enough to evaluate all generated terms of $\widehat{\Omega}^{(2)}$. As a result, the quantities $\Omega^{(2)\pm}$ are determined (Appendix C). Consequently, the restriction of space $\mathcal{P}$ the effective Hamiltonian $\widehat{\mathscr{H}}^{(3)}$ acts on to its subspaces $\mathcal{P}^{\Lambda}$ (see Eq. (4.4)) permits to express the expansion coefficients $\mathfrak{h}^{(3)}_{mn;\xi}$ in terms of $\Omega^{(2)\pm}$ (Tabs. 15-17). The key feature is that the coefficients $\Omega^{(2)\pm}$ can be replaced while on a particular case of interest, but the tensor structure of operators on $\mathcal{P}^{\Lambda}$ remains steady.

Tab. 18: The amount of one-body terms of $\widehat{\mathscr{H}}^{(3)}$

$(mn\xi)$	d^{+}	$\bar{d}^{+}$	d^{-}	$\bar{d}^{-}$
(111)	13	0	3	0
(122)	37	0	18	0
(212)	14	2	2	0
(223)	67	34	29	2
(234)	57	36	18	18
Total:	188	72	70	20

In total, there are computed $188+70 = 258$ direct one-body terms of $\widehat{\mathscr{H}}^{(3)}$ and $72+20 = 92$ direct one-body terms of $\widehat{\mathscr{H}}^{(3)}$ including the two-particle interactions g^0 only (in Tab. 18, the sign $\pm$ over d or $\bar{d}$ takes possession of the sign of $\widehat{h}^{(3)\pm}_{mn;\xi}$). To compare with, Blundell et. al. [41, Sec. II, Eq. (8)] calculated 84 diagrams contributing to the third-order mono-valent removal energy. Their studied energies $E^{(3)}_A$–$E^{(3)}_H$, $E^{(3)}_I$, $E^{(3)}_J$ and $E^{(3)}_K$, $E^{(3)}_L$ conform to the matrix elements of terms drawn in accordingly $\widehat{h}^{(3)}_{22;3}$, $\widehat{h}^{(3)}_{23;4}$ and $\widehat{h}^{(3)}_{21;2}$ if g^0 represents the Coulomb interaction. For instance, $E^{(3)}_A = \sum_{\mathrm{ee'c}} \widetilde{g}_{\mathrm{vce'e}}\, \omega^{(2)}_{\mathrm{ee'c\bar{v}}}$ which conforms to $\widetilde{z}(0\lambda_{\mathrm{v}}\lambda_{\mathrm{c}}\lambda_{\mu''}\lambda_{\mu'}\Lambda_1\Lambda_1)\Omega^{(2)}_{\mu'\mu''\mathrm{c}\bar{\mathrm{v}}}(\Lambda_1\Lambda_2\Lambda)$ pertained to $\mathfrak{h}^{(3)}_{22;3}(\Lambda)$ with $\mu = \mathrm{e}$ (Tab. 15).

Tab. 19 lists the amount of two-body terms of $\widehat{\mathscr{H}}^{(3)}$. There are computed $217 + 82 = 299$ direct two-body terms and $125 + 42 = 167$ direct two-body terms including the two-particle interactions g^0 only. For instance, Ho et. al. [37] calculated 218 two-body diagrams of the

Tab. 19: The amount of two-body terms of $\widehat{\mathscr{H}}^{(3)}$

$(mn\xi)$	d^+	$\bar{d}^+$	d^-	$\bar{d}^-$
(121)	20	0	10	0
(211)	13	2	3	0
(222)	64	32	31	4
(132)	20	16	10	10
(233)	75	50	28	28
(244)	25	25	–	–
Total:	217	125	82	42

third-order perturbation. Analogous disposition to account for the two-particle interactions g^0 only can be found and in other foremost works [36, 41].

At this step, it should be made an explanatory of such a comparison with other works. The principal difference of formulation of MBPT between the present and the other works is the difference between algebraic and diagrammatic realisation – all the rest of distinctive features follow the present one. Particularly, one of the typical features is the so-called factorisation theorem [37, Eq. (10)] which makes it possible to combine the diagrams with the same energy denominators. Consequently, the comparison of the amount of computed terms with the amount of computed diagrams is a very conditional one.

As it follows from Tab. 11, $\widehat{\mathscr{H}}^{(3)}$ also includes the terms $\widehat{h}^{(3)}_{mn;\xi}$ with $m+n-\xi = 0, 3, 4, 5$. The zero-body terms (the scalars on $\mathcal{P}^0$) are easy to derive. The result reads

$$\widehat{h}^{(3)+}_{11;2} = \sum_{\mathrm{c}} \sum_{\mu=\mathrm{v,e}} (-1)^{\lambda_\mu-\lambda_\mathrm{c}+m_0} f(\tau_0\lambda_\mathrm{c}\lambda_\mu)\Omega^{(2)+}_{\mu\mathrm{c}}(\tau_0), \tag{4.22a}$$

$$\widehat{h}^{(3)-}_{11;2} = \sum_{\mathrm{c}} \sum_{\mu=\mathrm{v,e}} f(\tau_0\lambda_\mathrm{c}\lambda_\mu)\Omega^{(2)-}_{\mu\mathrm{c}}(\tau_0), \tag{4.22b}$$

$$\begin{aligned}\widehat{h}^{(3)+}_{22;4} =& 2\sum_{\mathrm{cc'}}\sum_{\Lambda_1}\Bigg(\sum_{\mu=\mathrm{v,e}}(-1)^{\lambda_\mu+\lambda_{\mu'}}\Omega^{(2)+}_{\mu\mu'\mathrm{cc'}}(\Lambda_1\Lambda_1 0)\widetilde{z}(0\lambda_\mathrm{c}\lambda_{\mathrm{c'}}\lambda_{\mu'}\lambda_\mu\Lambda_1\Lambda_1) \\ &+ \sum_{\mathrm{v,e}} a(\lambda_\mathrm{e}\lambda_\mathrm{v}\Lambda_1)\Omega^{(2)+}_{\mathrm{evcc'}}(\Lambda_1\Lambda_1 0)\widetilde{z}(0\lambda_\mathrm{c}\lambda_{\mathrm{c'}}\lambda_\mathrm{v}\lambda_\mathrm{e}\Lambda_1\Lambda_1)\Bigg),\end{aligned} \tag{4.23a}$$

$$\begin{aligned}\widehat{h}^{(3)-}_{22;4} =& 2\sum_{\mathrm{cc'}}\sum_{\Lambda_1} a(\lambda_\mathrm{c}\lambda_{\mathrm{c'}}\Lambda_1)\Bigg(\sum_{\mu=\mathrm{v,e}}\Omega^{(2)-}_{\mu\mu'\mathrm{cc'}}(\Lambda_1\Lambda_1 0)\widetilde{z}(0\lambda_\mathrm{c}\lambda_{\mathrm{c'}}\lambda_{\mu'}\lambda_\mu\Lambda_1\Lambda_1) \\ &+ \sum_{\mathrm{v,e}}\Omega^{(2)-}_{\mathrm{evcc'}}(\Lambda_1\Lambda_1 0)\widetilde{z}(0\lambda_\mathrm{c}\lambda_{\mathrm{c'}}\lambda_\mathrm{v}\lambda_\mathrm{e}\Lambda_1\Lambda_1)\Bigg),\end{aligned} \tag{4.23b}$$

and $\widehat{h}^{(3)-}_{11;2}$ vanishes if the single-particle interactions v_i are neglected (see Eq. (C.1b) in Appendix C).

The study of excitations with $m+n-\xi > 2$ is usually much more complicated. However, once the SU(2)–invariant coefficients $\Omega^{(2)}$ are derived, the expansion coefficients $\mathfrak{h}^{(3)}_{mn;\xi}$ can be obtained in the same manner. In Ref. [42, Eqs. (19)-(20)], the triple excitations for $m = n = 2$, $\xi = 1$ have been considered. In this case,

$$\begin{aligned}\mathfrak{h}^{(3)+}_{22;1}(E_1\Lambda_1E_2\Lambda_2\Lambda) =& (-1)^{\lambda_{\mathrm{v}''}+\lambda_{\bar{\mathrm{v}}'}+\lambda_{\bar{\mathrm{v}}''}+\Lambda_2+\Lambda}[\Lambda_1,\Lambda_2]^{1/2}\sum_{\overline{\Lambda}_1}\Bigg(\sum_{\overline{\Lambda}_2}a(\lambda_{\mathrm{v}'}\lambda_{\bar{\mathrm{v}}}\overline{\Lambda}_2)[E_1,E_2,\overline{\Lambda}_1]^{1/2} \\ &\times\sum_{cu}\widetilde{z}(0\lambda_\mathrm{c}\lambda_\mathrm{v}\lambda_{\bar{\mathrm{v}}'}\lambda_{\bar{\mathrm{v}}}uu)\Omega^{(2)+}_{\mathrm{v'v''c\bar{v}''}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda)\begin{Bmatrix}\lambda_\mathrm{v} & \overline{\Lambda}_2 & \Lambda_2\\ \lambda_{\bar{\mathrm{v}}''} & u & \lambda_\mathrm{c}\end{Bmatrix}\begin{Bmatrix}\Lambda_2 & \lambda_\mathrm{v} & \overline{\Lambda}_2\\ \overline{\Lambda}_1 & \Lambda & \Lambda_1\end{Bmatrix}\begin{Bmatrix}\lambda_\mathrm{v} & \lambda_{\mathrm{v}'} & E_1\\ \lambda_{\mathrm{v}''} & \Lambda_1 & \overline{\Lambda}_1\end{Bmatrix}\begin{Bmatrix}\lambda_{\bar{\mathrm{v}}''} & \lambda_{\bar{\mathrm{v}}'} & E_2\\ \lambda_{\bar{\mathrm{v}}} & \Lambda_2 & u\end{Bmatrix} \\ &+(-1)^{E_1+E_2}\sum_{\mathrm{e}}\widetilde{z}(0\lambda_\mathrm{v}\lambda_{\mathrm{v}'}\lambda_\mathrm{e}\lambda_{\bar{\mathrm{v}}}E_1E_1)\Omega^{(2)+}_{\mathrm{ev''\bar{v}'\bar{v}''}}(\overline{\Lambda}_1E_2\Lambda)\begin{Bmatrix}\Lambda_1 & \overline{\Lambda}_1 & \lambda_{\bar{\mathrm{v}}}\\ \lambda_\mathrm{e} & E_1 & \lambda_{\mathrm{v}''}\end{Bmatrix}\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ E_2 & \overline{\Lambda}_1 & \lambda_{\bar{\mathrm{v}}}\end{Bmatrix}\Bigg),\end{aligned} \tag{4.24}$$

and the corresponding irreducible tensor operator in Eq. (4.4) is associated to the angular re-

duction scheme $\mathscr{T}_{12}^{[2^21^2]}$ so that

$$\widehat{O}_M^{\Lambda}([2^21^2]12) \equiv [[W^{E_1}(\lambda_{\mathrm{v}}\lambda_{\mathrm{v}'}) \times a^{\lambda_{\mathrm{v}}''}]^{\Lambda_1} \times [W^{E_2}(\widetilde{\lambda}_{\bar{\mathrm{v}}''}\widetilde{\lambda}_{\bar{\mathrm{v}}'}) \times \tilde{a}^{\lambda_{\bar{\mathrm{v}}}}]^{\Lambda_2}]_M^{\Lambda},$$

where $\widehat{h}_{22;1}^{(3)}$ contains 30 direct three-body terms of $\widehat{\mathscr{H}}^{(3)}$. The study of other expansion coefficients suitable for higher-order excitations is still in progress.

5 Prime results and conclusions

1. The RCGC technique based on the constituted $\mathrm{SO}(3)$–irreducible tensor operators has been originated. The key feature of proposed technique is the ability to reduce the N–electron angular integrals into the sum of single integrals. The method is especially convenient for the calculation of matrix elements of interaction operators on the basis of $\mathrm{SU}(2)$–irreducible matrix representations. As a result, the proposed technique makes it possible to turn to practical account the $\mathrm{SU}(2)$–irreducible matrix representations as a convenient basis rather than the usual Slater-type orbitals.

2. The effective operator approach has been developed. Based on the Feshbach's space partitioning technique, the finite-dimensional many-electron model space has been constructed. As a result, it has been determined that only a fixed number of types of the Hilbert space operators with respect to the single-electron states attach the non-zero effective operators on the given model space. The result has a consequential meaning in applications of atomic many-body perturbation theory, as it permits to reduce the number of expansion terms significantly.

3. A systematic way of inquiry of totally antisymmetric tensors has been brought to a more advanced state. Based on the S_ℓ–irreducible representations and the conception of tuples, the method to classify the angular reduction schemes of operator string of any length ℓ has been initiated. Based on the commutative diagrams that realise the mappings from a given angular reduction scheme to the required one, the permutation properties of antisymmetric tensors have been considered systematically. Special attention is paid to the case $\ell = 6$ which characterises the three-particle operators observed in the applications of effective operator approach to the atomic perturbation theory. As a result, the foundations developed for the irreducible tensor operators associated to distinct angular reduction schemes appear to be well-suited with respect to facility to compute the matrix representations of given operators.

4. The classification of three-particle operators that act on 2, 3, 4, 5, 6 electron shells of atom has been performed. The irreducible tensor operators associated to their own angular reduction schemes are identified by the classes. The classes are characterised by the number of electron shells the operator acts on and by the number of electrons in a given shell. The proposed classification is convenient to calculate the matrix elements of any three-particle operator. That is, the way of classification permits to establish the connection between the operators that belong to distinct classes, and thus it suffices to find the matrix representation for the sole operator – the matrix representations for the other operators are found instantly by using the transformation coefficients.

5. The third-order many-body perturbation theory has been considered. To simplify the generation of expansion terms followed by the generalised Bloch equation, the symbolic programming package *NCoperators* written on *Mathematica* has been produced. The angular reduction of generated terms has been performed making use of *NCoperators* too. The specific technique of reduction has been developed. The algorithm is based on the composed $\mathrm{SU}(2)$–invariants which—owed to the symmetry properties of matrix representations of atomic interaction operators—take into consideration all generated terms of the second-order wave operator. Therefore the irreducible tensor form of terms of the third-order effective Hamiltonian is applicable to other effective operator approaches used in MBPT: it is simply a manner of replacement of the excitation amplitudes suitable for some special cases of ones interests. Obtained symbolic preparation of terms of the third-order MBPT is convenient to implement it in the computer codes for the calculations of characteristic quantitites of atoms with several valence electrons as well.

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A Basis coefficients

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3\alpha_4(\alpha_{34})(\alpha_{1234}),\alpha_5\alpha_6(\alpha_{56})\alpha\right)\\
&=(-1)^{\wp_1}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\left[\alpha_{34},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{456},\alpha_{1234}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_6 & \alpha_5 & \alpha_{56}\\ \alpha_4 & \alpha_{456} & \alpha_{45}\end{Bmatrix}\begin{Bmatrix}\alpha_{12} & \alpha_3 & \alpha_{123}\\ \alpha_4 & \alpha_{1234} & \alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_{123} & \alpha_4 & \alpha_{1234}\\ \alpha_{56} & \alpha & \alpha_{456}\end{Bmatrix},
\end{aligned}\tag{A.1a}$$

$$\wp_1=\alpha_5+\alpha_6-\alpha_{56}+\alpha-\alpha_{12}+\alpha_{123}-\alpha_{1234}-\alpha_3-\alpha_4-\alpha_{456}.\tag{A.1b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3\alpha_4(\alpha_{34}),\alpha_5\alpha_6(\alpha_{56})(\alpha_{3456})\alpha\right)\\
&=(-1)^{\wp_2}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\left[\alpha_{34},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{456},\alpha_{3456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_6 & \alpha_5 & \alpha_{56}\\ \alpha_4 & \alpha_{456} & \alpha_{45}\end{Bmatrix}\begin{Bmatrix}\alpha_{12} & \alpha_3 & \alpha_{123}\\ \alpha_{456} & \alpha & \alpha_{3456}\end{Bmatrix}\begin{Bmatrix}\alpha_3 & \alpha_4 & \alpha_{34}\\ \alpha_{56} & \alpha_{3456} & \alpha_{456}\end{Bmatrix},
\end{aligned}\tag{A.2a}$$

$$\wp_2=\alpha_5+\alpha_6-\alpha_{56}+\alpha+\alpha_{12}+2\alpha_3+\alpha_{3456}.\tag{A.2b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3\alpha_4(\alpha_{34})(\alpha_{1234})\alpha_5(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_3}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\left[\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{456},\alpha_{1234},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{12} & \alpha_3 & \alpha_{123}\\ \alpha_4 & \alpha_{1234} & \alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_{12345} & \alpha_{123} & \alpha_{1234}\end{Bmatrix}\begin{Bmatrix}\alpha_{45} & \alpha_6 & \alpha_{456}\\ \alpha & \alpha_{123} & \alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.3a}$$

$$\wp_3=-\alpha_{45}+\alpha_{12345}-\alpha-\alpha_5+\alpha_6-\alpha_{12}-\alpha_{1234}-\alpha_3.\tag{A.3b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3\alpha_4(\alpha_{34})\alpha_5(\alpha_{345})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_4}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\left[\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{12} & \alpha_3 & \alpha_{123}\\ \alpha_{45} & \alpha_{12345} & \alpha_{345}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_{345} & \alpha_3 & \alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_{45} & \alpha_6 & \alpha_{456}\\ \alpha & \alpha_{123} & \alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.4a}$$

$$\wp_4=-\alpha_4-\alpha_5+\alpha_{345}-\alpha-\alpha_{12}-\alpha_{123}-\alpha_{12345}-\alpha_6.\tag{A.4b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3\alpha_4(\alpha_{34})\alpha_5(\alpha_{345})\alpha_6(\alpha_{3456})\alpha\right)\\
&=(-1)^{\wp_5}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\left[\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{3456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{12} & \alpha_3 & \alpha_{123}\\ \alpha_{456} & \alpha & \alpha_{3456}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_{345} & \alpha_3 & \alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_{45} & \alpha_6 & \alpha_{456}\\ \alpha_{3456} & \alpha_3 & \alpha_{345}\end{Bmatrix},
\end{aligned}\tag{A.5a}$$

$$\wp_5=-\alpha_3-\alpha_4+\alpha_5+\alpha_6+\alpha_{45}-\alpha_{12}+\alpha_{345}-\alpha_{456}-\alpha_{3456}-\alpha.\tag{A.5b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\right)\\
&=(-1)^{\wp_6}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\Delta\left(\alpha_{45},\alpha_6,\alpha_{456}\right)\Delta\left(\alpha_{123},\alpha_{456},\alpha\right)\left[\alpha_{12},\alpha_{23}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix},
\end{aligned}\tag{A.6a}$$

$$\wp_6=\alpha_1+\alpha_2+\alpha_3+\alpha_{123}.\tag{A.6b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_7}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{12},\alpha_{23},\alpha_{456},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_{45} & \alpha_6 & \alpha_{456}\\ \alpha & \alpha_{123} & \alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.7a}$$

$$\wp_7=\alpha_1+\alpha_2+\alpha_3-\alpha_6-\alpha_{45}-\alpha.\tag{A.7b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23}),\alpha_4\alpha_5(\alpha_{45})(\alpha_{2345})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_8}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{12},\alpha_{23},\alpha_{123},\alpha_{456},\alpha_{2345},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_3&\alpha_{123}&\alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_1&\alpha_{23}&\alpha_{123}\\\alpha_{45}&\alpha_{12345}&\alpha_{2345}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.8a}$$

$$\wp_8=\alpha_2+\alpha_3-\alpha_{12345}+2\alpha_1+\alpha_{23}+\alpha+\alpha_6.\tag{A.8b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23}),\alpha_4\alpha_5(\alpha_{45})(\alpha_{2345})\alpha_6(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_9}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{12},\alpha_{23},\alpha_{123},\alpha_{456},\alpha_{2345},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_3&\alpha_{123}&\alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_1&\alpha_{23}&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha_{23456}&\alpha_{23}&\alpha_{2345}\end{Bmatrix},
\end{aligned}\tag{A.9a}$$

$$\wp_9=\alpha_2+\alpha_3+\alpha_{123}+\alpha_{23456}+\alpha_6+\alpha_{45}-\alpha_{456}-\alpha.\tag{A.9b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{10}}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\Delta\left(\alpha_{45},\alpha_6,\alpha_{456}\right)\left[\alpha_{12},\alpha_{23},\alpha_{123},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_3&\alpha_{123}&\alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_1&\alpha_{23}&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{23456}\end{Bmatrix},
\end{aligned}\tag{A.10a}$$

$$\wp_{10}=\alpha-\alpha_{123}+\alpha_2-\alpha_{23}+\alpha_3+\alpha_{456}.\tag{A.10b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})(\alpha_{234})(\alpha_{1234}),\alpha_5\alpha_6(\alpha_{56})\alpha\right)\\
&=(-1)^{\wp_{11}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{456},\alpha_{234},\alpha_{1234}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{34}&\alpha_{1234}&\alpha_{234}\end{Bmatrix}\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_4&\alpha_{1234}&\alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_6&\alpha_{456}&\alpha_{56}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_{56}&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{1234}\end{Bmatrix},
\end{aligned}\tag{A.11a}$$

$$\wp_{11}=-\alpha_1+\alpha_2+\alpha_3+\alpha_{12}+\alpha_{34}+\alpha_5+\alpha_6-\alpha_{56}+\alpha_{456}-\alpha_4-\alpha_{123}-\alpha.\tag{A.11b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})(\alpha_{234}),\alpha_5\alpha_6(\alpha_{56})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{12}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_6&\alpha_{456}&\alpha_{56}\end{Bmatrix}\begin{bmatrix}\alpha_2&\alpha_{23456}&\alpha_3&\alpha_{456}\\\alpha_{12}&\alpha_{34}&\alpha&\alpha_{56}\\\alpha_1&\alpha_{123}&\alpha_{234}&\alpha_4\end{bmatrix},
\end{aligned}\tag{A.12a}$$

$$\wp_{12}=\alpha_5+\alpha_6-\alpha_{123}-\alpha_4-\alpha_{234}+\alpha_{23456}+\alpha_{12}-\alpha_{34}.\tag{A.12b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34}),\alpha_5\alpha_6(\alpha_{56})(\alpha_{3456})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{13}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{456},\alpha_{3456},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{3456}&\alpha&\alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{3456}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_6&\alpha_{456}&\alpha_{56}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_{56}&\alpha_{456}\\\alpha_{3456}&\alpha_3&\alpha_{34}\end{Bmatrix},
\end{aligned}\tag{A.13a}$$

$$\wp_{13}=\alpha_5+\alpha_6-\alpha_{56}-\alpha_1-\alpha_2+\alpha_{12}+2\alpha_3.\tag{A.13b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\right)\\
&=\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_{12},\alpha_3,\alpha_{123}\right)\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\Delta\left(\alpha_{45},\alpha_6,\alpha_{456}\right)\\
&\times\Delta\left(\alpha_{123},\alpha_{456},\alpha\right).
\end{aligned}\tag{A.14}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{15}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_{12},\alpha_3,\alpha_{123}\right)\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{456},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.15a}$$

$$\wp_{15}=\alpha+\alpha_{123}+\alpha_6+\alpha_{45}.\tag{A.15b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3,\alpha_4\alpha_5(\alpha_{45})(\alpha_{345})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{16}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{45}&\alpha_{12345}&\alpha_{345}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.16a}$$

$$\wp_{16}=\alpha-\alpha_{12}+\alpha_{123}-\alpha_{12345}-\alpha_3+\alpha_6.\tag{A.16b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3,\alpha_4\alpha_5(\alpha_{45})(\alpha_{345})\alpha_6(\alpha_{3456})\alpha\right)\\
&=(-1)^{\wp_{17}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{3456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{3456}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha_{3456}&\alpha_3&\alpha_{345}\end{Bmatrix},
\end{aligned}\tag{A.17a}$$

$$\wp_{17}=\alpha+\alpha_{12}-\alpha_{3456}+\alpha_{45}-\alpha_{456}+\alpha_6.\tag{A.17b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3,\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})(\alpha_{3456})\alpha\right)\\
&=(-1)^{\wp_{18}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\Delta\left(\alpha_{45},\alpha_6,\alpha_{456}\right)\left[\alpha_{123},\alpha_{3456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{3456}\end{Bmatrix},
\end{aligned}\tag{A.18a}$$

$$\wp_{18}=\alpha+\alpha_{12}+\alpha_3+\alpha_{456}.\tag{A.18b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4,\alpha_5\alpha_6(\alpha_{56})(\alpha_{456})\alpha\right)\\
&=(-1)^{\wp_{19}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_{12},\alpha_3,\alpha_{123}\right)\Delta\left(\alpha_{123},\alpha_{456},\alpha\right)\left[\alpha_{45},\alpha_{56}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_6&\alpha_{456}&\alpha_{56}\end{Bmatrix},
\end{aligned}\tag{A.19a}$$

$$\wp_{19}=\alpha_4+\alpha_5+\alpha_6+\alpha_{456}.\tag{A.19b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123})\alpha_4(\alpha_{1234}),\alpha_5\alpha_6(\alpha_{56})\alpha\right)\\
&=(-1)^{\wp_{20}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_{12},\alpha_3,\alpha_{123}\right)\left[\alpha_{45},\alpha_{56},\alpha_{456},\alpha_{1234}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_6&\alpha_{456}&\alpha_{56}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_{56}&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{1234}\end{Bmatrix},
\end{aligned}\tag{A.20a}$$

$$\wp_{20}=\alpha+\alpha_{123}-\alpha_{456}+\alpha_5+\alpha_6-\alpha_{56}.\tag{A.20b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12}),\alpha_3,\alpha_4,\alpha_5\alpha_6(\alpha_{56})(\alpha_{456})(\alpha_{3456})\alpha\right)\\
&=(-1)^{\wp_{21}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\left[\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{3456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_6&\alpha_{456}&\alpha_{56}\end{Bmatrix}\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{3456}\end{Bmatrix},
\end{aligned}\tag{A.21a}$$

$$\wp_{21}=-\alpha_3+\alpha_4+\alpha_5+\alpha_6-\alpha_{12}-\alpha.\tag{A.21b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})(\alpha_{123}),\alpha_4,\alpha_5\alpha_6(\alpha_{56})(\alpha_{456})\alpha\right)\\
&=(-1)^{\wp_{22}}\Delta\left(\alpha_{123},\alpha_{456},\alpha\right)\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{56}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_6 & \alpha_{456} & \alpha_{56}\end{Bmatrix},
\end{aligned}\tag{A.22a}$$

$$\wp_{22}=\alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6+\alpha_{123}+\alpha_{456}.\tag{A.22b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})(\alpha_{123})\alpha_4(\alpha_{1234}),\alpha_5\alpha_6(\alpha_{56})\alpha\right)\\
&=(-1)^{\wp_{23}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{56},\alpha_{456},\alpha_{1234}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_6 & \alpha_{456} & \alpha_{56}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_{56} & \alpha_{456}\\ \alpha & \alpha_{123} & \alpha_{1234}\end{Bmatrix},
\end{aligned}\tag{A.23a}$$

$$\wp_{23}=\alpha_1+\alpha_2+\alpha_3+\alpha_5+\alpha_6-\alpha_{56}-\alpha+\alpha_{456}.\tag{A.23b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})\alpha_4(\alpha_{234})(\alpha_{1234}),\alpha_5\alpha_6(\alpha_{56})\alpha\right)\\
&=(-1)^{\wp_{24}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{1234}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_1 & \alpha_{23} & \alpha_{123}\\ \alpha_4 & \alpha_{1234} & \alpha_{234}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_6 & \alpha_{456} & \alpha_{56}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_{56} & \alpha_{456}\\ \alpha & \alpha_{123} & \alpha_{1234}\end{Bmatrix},
\end{aligned}\tag{A.24a}$$

$$\wp_{24}=\alpha_2+\alpha_3-\alpha_4+\alpha_5+\alpha_6-\alpha_{23}-\alpha_{56}+\alpha_{456}-\alpha-\alpha_{1234}.\tag{A.24b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})\alpha_4(\alpha_{234}),\alpha_5\alpha_6(\alpha_{56})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{25}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_1 & \alpha_{23} & \alpha_{123}\\ \alpha_{456} & \alpha & \alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_6 & \alpha_{456} & \alpha_{56}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_{56} & \alpha_{456}\\ \alpha_{23456} & \alpha_{23} & \alpha_{234}\end{Bmatrix},
\end{aligned}\tag{A.25a}$$

$$\wp_{25}=\alpha_2+\alpha_3-\alpha_{123}+\alpha_5+\alpha_6-\alpha_{56}+\alpha+\alpha_{23456}.\tag{A.25b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23}),\alpha_4,\alpha_5\alpha_6(\alpha_{56})(\alpha_{456})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{26}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{56},\alpha_{123},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_1 & \alpha_{23} & \alpha_{123}\\ \alpha_{456} & \alpha & \alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_6 & \alpha_{456} & \alpha_{56}\end{Bmatrix},
\end{aligned}\tag{A.26a}$$

$$\wp_{26}=\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6-\alpha_{23}+\alpha_{123}-\alpha.\tag{A.26b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123})\alpha_4(\alpha_{1234})\alpha_5(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{27}}\Delta\left(\alpha_1,\alpha_2,\alpha_{12}\right)\Delta\left(\alpha_{12},\alpha_3,\alpha_{123}\right)\left[\alpha_{45},\alpha_{456},\alpha_{1234},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_{12345} & \alpha_{123} & \alpha_{1234}\end{Bmatrix}\begin{Bmatrix}\alpha_{45} & \alpha_6 & \alpha_{456}\\ \alpha & \alpha_{123} & \alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.27a}$$

$$\wp_{27}=-\alpha+\alpha_{12345}+\alpha_4+\alpha_5-\alpha_6-\alpha_{45}.\tag{A.27b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})(\alpha_{123})\alpha_4(\alpha_{1234})\alpha_5(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{28}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{456},\alpha_{1234},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1 & \alpha_2 & \alpha_{12}\\ \alpha_3 & \alpha_{123} & \alpha_{23}\end{Bmatrix}\begin{Bmatrix}\alpha_4 & \alpha_5 & \alpha_{45}\\ \alpha_{12345} & \alpha_{123} & \alpha_{1234}\end{Bmatrix}\begin{Bmatrix}\alpha_{45} & \alpha_6 & \alpha_{456}\\ \alpha & \alpha_{123} & \alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.28a}$$

$$\wp_{28}=\alpha_1+\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6+\alpha_{45}-\alpha_{123}+\alpha+\alpha_{12345}.\tag{A.28b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})\alpha_4(\alpha_{234})(\alpha_{1234})\alpha_5(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{29}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{1234},\alpha_{12345}\right]^{\frac{1}{2}}\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_3&\alpha_{123}&\alpha_{23}\end{Bmatrix}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_{23}&\alpha_{123}\\\alpha_4&\alpha_{1234}&\alpha_{234}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_{12345}&\alpha_{123}&\alpha_{1234}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.29a}$$

$$\wp_{29}=\alpha_2+\alpha_3-\alpha_{23}+\alpha_{123}+\alpha_{1234}+\alpha_{12345}+\alpha-\alpha_5+\alpha_6-\alpha_{45}.\tag{A.29b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})\alpha_4(\alpha_{234})\alpha_5(\alpha_{2345})\alpha_6(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{30}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{2345},\alpha_{23456}\right]^{\frac{1}{2}}\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_3&\alpha_{123}&\alpha_{23}\end{Bmatrix}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_{23}&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_{2345}&\alpha_{23}&\alpha_{234}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha_{23456}&\alpha_{23}&\alpha_{2345}\end{Bmatrix},
\end{aligned}\tag{A.30a}$$

$$\wp_{30}=\alpha_2+\alpha_3+\alpha_4+\alpha_5+\alpha_6-\alpha_{23}-\alpha_{45}-\alpha_{123}-\alpha_{2345}+\alpha+\alpha_{23456}+\alpha_{456}.\tag{A.30b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2\alpha_3(\alpha_{23})\alpha_4(\alpha_{234})\alpha_5(\alpha_{2345})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{31}}\left[\alpha_{12},\alpha_{23},\alpha_{45},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{2345},\alpha_{12345}\right]^{\frac{1}{2}}\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_3&\alpha_{123}&\alpha_{23}\end{Bmatrix}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_{23}&\alpha_{123}\\\alpha_{45}&\alpha_{12345}&\alpha_{2345}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_{2345}&\alpha_{23}&\alpha_{234}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.31a}$$

$$\wp_{31}=\alpha_2+\alpha_3-\alpha_4-\alpha_5+\alpha_6+\alpha_{2345}+\alpha+\alpha_{12345}.\tag{A.31b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})(\alpha_{234})(\alpha_{1234})\alpha_5(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{32}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{1234},\alpha_{12345}\right]^{\frac{1}{2}}\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{34}&\alpha_{1234}&\alpha_{234}\end{Bmatrix}\\
&\times\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_4&\alpha_{1234}&\alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_{12345}&\alpha_{123}&\alpha_{1234}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.32a}$$

$$\wp_{32}=\alpha_1+\alpha_2+\alpha_{34}+\alpha_6+\alpha_{45}+\alpha+\alpha_5+\alpha_{12345}+\alpha_3+\alpha_{12}.\tag{A.32b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})(\alpha_{234})\alpha_5(\alpha_{2345})\alpha_6(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{33}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{2345},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{bmatrix}\alpha_1&&\alpha_2&&\alpha_{234}&&\alpha_{2345}&&\alpha_{23456}&\\&\alpha_{12}&&\alpha_{34}&&\alpha_5&&\alpha_6&&\alpha\\\alpha_{123}&&\alpha_3&&\alpha_4&&\alpha_{45}&&\alpha_{456}&\end{bmatrix},
\end{aligned}\tag{A.33a}$$

$$\wp_{33}=\alpha_1+\alpha_2-\alpha_{12}+\alpha_{34}-\alpha_3-\alpha_4.\tag{A.33b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})(\alpha_{234})\alpha_5(\alpha_{2345})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{34}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{234},\alpha_{456},\alpha_{2345},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix}\begin{bmatrix}\alpha_2&\alpha_{2345}&\alpha_3&\alpha_{45}\\\alpha_{12}&\alpha_{34}&\alpha_{12345}&\alpha_5\\\alpha_1&\alpha_{123}&\alpha_{234}&\alpha_4\end{bmatrix},
\end{aligned}\tag{A.34a}$$

$$\wp_{34}=-\alpha_{234}+\alpha_{2345}+2\alpha_4+\alpha+\alpha_6+\alpha_{12}-\alpha_{34}.\tag{A.34b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})\alpha_5(\alpha_{345})\alpha_6(\alpha_{3456})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{35}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{3456},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{3456}&\alpha&\alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{3456}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_{345}&\alpha_3&\alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha_{3456}&\alpha_3&\alpha_{345}\end{Bmatrix},
\end{aligned}\tag{A.35a}$$

$$\wp_{35}=\alpha_{345}-\alpha_3+\alpha_4+\alpha_5+\alpha_{45}+\alpha_6+\alpha_{456}-\alpha_1-\alpha_2+\alpha_{12}.\tag{A.35b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})\alpha_5(\alpha_{345})(\alpha_{2345})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{36}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{2345},\alpha_{12345}\right]^{\frac{1}{2}}\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{345}&\alpha_{12345}&\alpha_{2345}\end{Bmatrix}\\
&\times\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{45}&\alpha_{12345}&\alpha_{345}\end{Bmatrix}\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_{345}&\alpha_3&\alpha_{34}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.36a}$$

$$\wp_{36}=\alpha_1+\alpha_2-\alpha_4-\alpha_5+\alpha+\alpha_{12}-\alpha_{123}+\alpha_6.\tag{A.36b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3\alpha_4(\alpha_{34})\alpha_5(\alpha_{345})(\alpha_{2345})\alpha_6(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{37}}\left[\alpha_{12},\alpha_{34},\alpha_{45},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{2345},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_4&\alpha_5&\alpha_{45}\\\alpha_{345}&\alpha_3&\alpha_{34}\end{Bmatrix}\begin{bmatrix}\alpha_2&\alpha_{23456}&\alpha_3&\alpha_{456}\\\alpha_{12}&\alpha_{345}&\alpha&\alpha_6\\\alpha_1&\alpha_{123}&\alpha_{2345}&\alpha_{45}\end{bmatrix},
\end{aligned}\tag{A.37a}$$

$$\wp_{37}=\alpha_4+\alpha_5+\alpha_{2345}-\alpha_{123}+\alpha_3-\alpha_{23456}+\alpha_{456}+\alpha_{12}.\tag{A.37b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3,\alpha_4\alpha_5(\alpha_{45})(\alpha_{345})\alpha_6(\alpha_{3456})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{38}}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{12},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{3456},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{3456}&\alpha&\alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{3456}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha_{3456}&\alpha_3&\alpha_{345}\end{Bmatrix},
\end{aligned}\tag{A.38a}$$

$$\wp_{38}=\alpha_6+\alpha_{45}-\alpha_{456}+2\alpha-\alpha_1-\alpha_2-\alpha_{12}.\tag{A.38b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3,\alpha_4\alpha_5(\alpha_{45})(\alpha_{345})(\alpha_{2345})(\alpha_{12345})\alpha_6\alpha\right)\\
&=(-1)^{\wp_{39}}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{12},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{2345},\alpha_{12345}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{345}&\alpha_{12345}&\alpha_{2345}\end{Bmatrix}\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{45}&\alpha_{12345}&\alpha_{345}\end{Bmatrix}\begin{Bmatrix}\alpha_{45}&\alpha_6&\alpha_{456}\\\alpha&\alpha_{123}&\alpha_{12345}\end{Bmatrix},
\end{aligned}\tag{A.39a}$$

$$\wp_{39}=\alpha_1+\alpha_2+\alpha_{345}+\alpha-\alpha_{12}+\alpha_{123}-\alpha_3+\alpha_6.\tag{A.39b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3,\alpha_4\alpha_5(\alpha_{45})(\alpha_{345})(\alpha_{2345})\alpha_6(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{40}}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\left[\alpha_{12},\alpha_{123},\alpha_{345},\alpha_{456},\alpha_{2345},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{bmatrix}\alpha_1&\alpha_{2345}&\alpha_{123}&\alpha_{45}\\\alpha_{12}&\alpha&\alpha_{345}&\alpha_6\\\alpha_2&\alpha_3&\alpha_{23456}&\alpha_{456}\end{bmatrix},
\end{aligned}\tag{A.40a}$$

$$\wp_{40}=\alpha_{123}+\alpha_{2345}+2\alpha_2+\alpha_{23456}-\alpha_{456}-\alpha_{12}-\alpha_{345}.\tag{A.40b}$$

$$\begin{aligned}
&\left(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}),\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha\middle|\alpha_1,\alpha_2,\alpha_3,\alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})(\alpha_{3456})(\alpha_{23456})\alpha\right)\\
&=(-1)^{\wp_{41}}\Delta\left(\alpha_4,\alpha_5,\alpha_{45}\right)\Delta\left(\alpha_{45},\alpha_6,\alpha_{456}\right)\left[\alpha_{12},\alpha_{123},\alpha_{3456},\alpha_{23456}\right]^{\frac{1}{2}}\\
&\times\begin{Bmatrix}\alpha_1&\alpha_2&\alpha_{12}\\\alpha_{3456}&\alpha&\alpha_{23456}\end{Bmatrix}\begin{Bmatrix}\alpha_{12}&\alpha_3&\alpha_{123}\\\alpha_{456}&\alpha&\alpha_{3456}\end{Bmatrix},
\end{aligned}\tag{A.41a}$$

$$\wp_{41}=\alpha_{12}-\alpha_1-\alpha_2+\alpha_3+\alpha_{456}-\alpha_{3456}.\tag{A.41b}$$

$$\begin{aligned}
&\big(\alpha_1\alpha_2(\alpha_{12})\alpha_3(\alpha_{123}), \alpha_4\alpha_5(\alpha_{45})\alpha_6(\alpha_{456})\alpha \big| \alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5\alpha_6(\alpha_{56})(\alpha_{456})(\alpha_{3456})(\alpha_{23456})\alpha\big) \\
&= (-1)^{\wp_{42}} \left[\alpha_{12}, \alpha_{45}, \alpha_{56}, \alpha_{123}, \alpha_{3456}, \alpha_{23456}\right]^{\frac{1}{2}} \\
&\times \begin{Bmatrix} \alpha_1 & \alpha_2 & \alpha_{12} \\ \alpha_{3456} & \alpha & \alpha_{23456} \end{Bmatrix} \begin{Bmatrix} \alpha_{12} & \alpha_3 & \alpha_{123} \\ \alpha_{456} & \alpha & \alpha_{3456} \end{Bmatrix} \begin{Bmatrix} \alpha_4 & \alpha_5 & \alpha_{45} \\ \alpha_6 & \alpha_{456} & \alpha_{56} \end{Bmatrix}, \qquad \text{(A.42a)} \\
&\wp_{42} = -\alpha_4 - \alpha_5 - \alpha_6 + \alpha_{12} - \alpha_1 - \alpha_2 + \alpha_3 - \alpha_{3456}. \qquad \text{(A.42b)}
\end{aligned}$$

B The classification of three-particle operators acting on $\ell = 2, 3, 4, 5, 6$ electron shells

B.1 2–shell case

Tab. 20: The class $X_2\,(0, 0)$: $d_2 = 12$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 112112 \rangle$	(35)	$\langle 111122 \rangle$
$\langle 121112 \rangle$	(25)	
$\langle 211112 \rangle$	(15)	
$\langle 121121 \rangle$	(26)	
$\langle 112121 \rangle$	(36)	
$\langle 112211 \rangle$	(35) (46)	
$\langle 122122 \rangle$	(24)	$\langle 112222 \rangle$
$\langle 122212 \rangle$	(25)	
$\langle 122221 \rangle$	(26)	
$\langle 212122 \rangle$	(14)	
$\langle 212212 \rangle$	(15)	
$\langle 221122 \rangle$	(13) (24)	

Tab. 21: The class $X_2\,(+1, -1)$: $d_2 = 15$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 111112 \rangle$	1_6	$\langle 111112 \rangle$
$\langle 111121 \rangle$	(56)	
$\langle 111211 \rangle$	(46)	
$\langle 211122 \rangle$	(14)	$\langle 111222 \rangle$
$\langle 121122 \rangle$	(24)	
$\langle 112122 \rangle$	(34)	
$\langle 211212 \rangle$	(15)	
$\langle 121212 \rangle$	(25)	$\langle 111222 \rangle$
$\langle 112212 \rangle$	(35)	
$\langle 211221 \rangle$	(16)	
$\langle 121221 \rangle$	(26)	
$\langle 112221 \rangle$	(36)	
$\langle 122222 \rangle$	1_6	$\langle 122222 \rangle$
$\langle 212222 \rangle$	(12)	
$\langle 221222 \rangle$	(13)	

Tab. 22: The class $X_2\,(+2, -2)$: $d_2 = 6$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 111122 \rangle$	1_6	$\langle 111122 \rangle$
$\langle 111212 \rangle$	(45)	
$\langle 111221 \rangle$	(46)	
$\langle 112222 \rangle$	1_6	$\langle 112222 \rangle$
$\langle 121222 \rangle$	(23)	
$\langle 211222 \rangle$	(13)	

The class $X_2(+3, -3)$ contains the sole operator associated to the scheme $\langle x_\pi \rangle = \langle 111222 \rangle$ with $\pi = 1_6$.

B.2 3–shell case

Tab. 23: The class $X_3\,(0, 0, 0)$: $d_3 = 21$

$\langle x_\pi \rangle$	π	$\langle x \rangle$	$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 123\,\{123\} \rangle$	(24) (35) ϑ	$\langle 112233 \rangle$	$\langle 213213 \rangle$	(135)	$\langle 112233 \rangle$
$\langle 132123 \rangle$	(254)		$\langle 213312 \rangle$	(135) (46)	
$\langle 132132 \rangle$	(264)		$\langle 231123 \rangle$	(13) (254)	
$\langle 132213 \rangle$	(25)		$\langle 231132 \rangle$	(13) (264)	
$\langle 132231 \rangle$	(26)		$\langle 231213 \rangle$	(13) (25)	
$\langle 132312 \rangle$	(25) (46)		$\langle 312123 \rangle$	(154)	
$\langle 213123 \rangle$	(14) (35)		$\langle 312213 \rangle$	(15)	
$\langle 213132 \rangle$	(14) (36)		$\langle 321123 \rangle$	(154) (23)	

Tab. 24: The class $X_3\,(+2,-1,-1)$: $d_3 = 24$

$\langle x_\pi \rangle$	π	$\langle x \rangle$	$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 111\,\{123\}\rangle$	ϑ	$\langle 111123\rangle$	$\langle 113233\rangle$	(34)	$\langle 112333\rangle$
$\langle 112223\rangle$	1_6	$\langle 112223\rangle$	$\langle 113323\rangle$	(35)	
$\langle 112232\rangle$	(56)		$\langle 113332\rangle$	(36)	
$\langle 112322\rangle$	(46)		$\langle 131233\rangle$	(243)	
$\langle 121223\rangle$	(23)		$\langle 131323\rangle$	(253)	
$\langle 121232\rangle$	$(23)\,(56)$		$\langle 131332\rangle$	(263)	
$\langle 121322\rangle$	$(23)\,(46)$		$\langle 311233\rangle$	(143)	
$\langle 211223\rangle$	(13)		$\langle 311323\rangle$	(153)	
$\langle 211232\rangle$	$(13)\,(56)$		$\langle 311332\rangle$	(163)	
$\langle 211322\rangle$	$(13)\,(46)$				
	$X_3(-1,+2,-1)$:			$X_3(-1,-1,+2)$:	
$\langle x \rangle$	$\tilde{\pi}$	$\langle y \rangle$	$\langle x \rangle$	$\tilde{\pi}$	$\langle y \rangle$
$\langle 111123\rangle$	(15)	$\langle 122223\rangle$	$\langle 111123\rangle$	$(16)\,(25)$	$\langle 123333\rangle$
$\langle 112223\rangle$	$(14)\,(25)$	$\langle 111223\rangle$	$\langle 112223\rangle$	$(16)\,(25)$	$\langle 122233\rangle$
$\langle 112333\rangle$	(13)	$\langle 122333\rangle$	$\langle 112333\rangle$	$(16)\,(25)$	$\langle 111233\rangle$

Tab. 25: The class $X_3\,(+3,-2,-1)$: $d_3 = 3$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 111223\rangle$	1_6	$\langle 111223\rangle$
$\langle 111232\rangle$	(56)	
$\langle 111322\rangle$	$-\,(46)$	
Derived classes	$\tilde{\pi}$	$\langle y \rangle$
$X_3\,(-2,+3,-1)$	$(15)\,(24)$	$\langle 112223\rangle$
$X_3\,(-1,-2,+3)$	$(16)\,(24)\,(35)$	$\langle 122333\rangle$
$X_3\,(+3,-1,-2)$	(46)	$\langle 111233\rangle$
$X_3\,(-1,+3,-2)$	(146)	$\langle 122233\rangle$
$X_3\,(-2,-1,+3)$	$(14)\,(25)\,(36)$	$\langle 112333\rangle$

Tab. 26: The class $X_3\,(+1,-1,0)$: $d_3 = 45$

$\langle x_\pi \rangle$	π	$\langle x \rangle$	$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 133233\rangle$	(24)	$\langle 123333\rangle$	$\langle 313332\rangle$	(162)	$\langle 123333\rangle$
$\langle 133323\rangle$	(25)		$\langle 331233\rangle$	$(13)\,(24)$	
$\langle 133332\rangle$	(26)		$\langle 331323\rangle$	$(13)\,(25)$	
$\langle 313233\rangle$	(142)		$\langle 331332\rangle$	$(13)\,(26)$	
$\langle 313323\rangle$	(152)				
$\langle 113\,\{123\}\rangle$	$(354)\,\vartheta$	$\langle 111233\rangle$	$\langle\{123\}\,223\rangle$	$(35)\,\eta$	$\langle 122233\rangle$
$\langle 131\,\{123\}\rangle$	$(254)\,\vartheta$		$\langle\{123\}\,232\rangle$	$(36)\,\eta$	
$\langle 311\,\{123\}\rangle$	$(154)\,\vartheta$		$\langle\{123\}\,322\rangle$	$(35)\,(46)\,\eta$	
	$X_3\,(+1,0,-1)$:			$X_3\,(0,+1,-1)$:	
$\langle x \rangle$	$\tilde{\pi}$	$\langle y \rangle$	$\langle x \rangle$	$\tilde{\pi}$	$\langle y \rangle$
$\langle 123333\rangle$	(162)	$\langle 122223\rangle$	$\langle 123333\rangle$	$(15)\,(26)$	$\langle 111123\rangle$
$\langle 111233\rangle$	(46)	$\langle 111223\rangle$	$\langle 111233\rangle$	$(15)\,(246)$	$\langle 112223\rangle$
$\langle 122233\rangle$	$(25)\,(36)$	$\langle 122333\rangle$	$\langle 122233\rangle$	$(135)\,(26)$	$\langle 112333\rangle$

Tab. 27: The class $X_3\,(+2,-2,0)$: $d_3 = 9$

$\langle x_\pi \rangle$	π	$\langle x \rangle$	$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 113223\rangle$	(35)	$\langle 112233\rangle$	$\langle 131322\rangle$	$(253)\,(46)$	$\langle 112233\rangle$
$\langle 113232\rangle$	(36)		$\langle 311223\rangle$	(153)	
$\langle 113322\rangle$	$(35)\,(46)$		$\langle 311232\rangle$	(163)	
$\langle 131223\rangle$	(253)		$\langle 311322\rangle$	$(153)\,(46)$	
$\langle 131232\rangle$	(263)				
Derived class	$\tilde{\pi}$	$\langle y \rangle$	*Derived class*	$\tilde{\pi}$	$\langle y \rangle$
$X_3\,(+2,0,-2)$	$(35)\,(46)$	$\langle 112233\rangle$	$X_3\,(0,+2,-2)$	$(135)\,(246)$	$\langle 112233\rangle$

B.3 4–shell case

Tab. 28: The class $X_4\,(+1, +1, -1, -1)$: $d_4 = 72$

$\langle x_\pi \rangle$	π	$\langle x \rangle$	$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 112\,\{134\}\rangle$	$(34)\,\vartheta$	$\langle 111234\rangle$	$\langle 122\,\{234\}\rangle$	ϑ	$\langle 122234\rangle$
$\langle 121\,\{134\}\rangle$	$(24)\,\vartheta$		$\langle 212\,\{234\}\rangle$	$(12)\,\vartheta$	
$\langle 211\,\{134\}\rangle$	$(14)\,\vartheta$		$\langle 221\,\{234\}\rangle$	$(13)\,\vartheta$	
$\langle\{123\}\,334\rangle$	η	$\langle 123334\rangle$	$\langle\{124\}\,344\rangle$	$(34)\,\eta$	$\langle 123444\rangle$
$\langle\{123\}\,343\rangle$	$(56)\,\eta$		$\langle\{124\}\,434\rangle$	$(35)\,\eta$	
$\langle\{123\}\,433\rangle$	$(46)\,\eta$		$\langle\{124\}\,443\rangle$	$(36)\,\eta$	
	$X_4\,(+1, -1, +1, -1)$:			$X_4\,(+1, -1, -1, +1)$:	
$\langle x \rangle$	$\tilde{\pi}$	$\langle y \rangle$	$\langle x \rangle$	$\tilde{\pi}$	$\langle y \rangle$
$\langle 111234\rangle$	(45)	$\langle 111234\rangle$	$\langle 111234\rangle$	(46)	$\langle 111234\rangle$
$\langle 122234\rangle$	(25)	$\langle 123334\rangle$	$\langle 122234\rangle$	$(26)\,(35)$	$\langle 123444\rangle$
$\langle 123334\rangle$	(25)	$\langle 122234\rangle$	$\langle 123334\rangle$	(26)	$\langle 123334\rangle$
$\langle 123444\rangle$	(23)	$\langle 123444\rangle$	$\langle 123444\rangle$	$(26)\,(35)$	$\langle 122234\rangle$

Tab. 29: The class $X_4\,(+2, -2, +1, -1)$: $d_4 = 9$

$\langle x_\pi \rangle$	π	$\langle x \rangle$	$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 113224\rangle$	(35)	$\langle 112234\rangle$	$\langle 131422\rangle$	$(253)\,(46)$	$\langle 112234\rangle$
$\langle 113242\rangle$	(356)		$\langle 311224\rangle$	(1532)	
$\langle 113422\rangle$	$(35)\,(46)$		$\langle 311242\rangle$	(1563)	
$\langle 131224\rangle$	(253)		$\langle 311422\rangle$	$(153)\,(46)$	
$\langle 131242\rangle$	(2563)				
Derived classes	$\tilde{\pi}$	$\langle y \rangle$	*Derived classes*	$\tilde{\pi}$	$\langle y \rangle$
$X_4\,(+2, -2, -1, +1)$	(56)	$\langle 112234\rangle$	$X_4\,(+1, +2, -2, -1)$	(135)	$\langle 122334\rangle$
$X_4\,(+2, +1, -2, -1)$	(35)	$\langle 112334\rangle$	$X_4\,(+1, +2, -1, -2)$	$(135)\,(46)$	$\langle 122344\rangle$
$X_4\,(+2, +1, -1, -2)$	$(35)\,(46)$	$\langle 112344\rangle$	$X_4\,(+1, -2, +2, -1)$	$(15)\,(24)$	$\langle 122334\rangle$
$X_4\,(+2, -1, -2, +1)$	(356)	$\langle 112334\rangle$	$X_4\,(+1, -2, -1, +2)$	$(15)\,(264)$	$\langle 122344\rangle$
$X_4\,(+2, -1, +1, -2)$	$(36)\,(45)$	$\langle 112344\rangle$	$X_4\,(+1, -1, +2, -2)$	$(135)\,(246)$	$\langle 123344\rangle$
			$X_4\,(+1, -1, -2, +2)$	$(15)\,(26)$	$\langle 123344\rangle$

Tab. 30: The class $X_4\,(+3, -1, -1, -1)$: $d_4 = 6$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 111\,\{234\}\rangle$	ϑ	$\langle 111234\rangle$
Derived classes	$\tilde{\pi}$	$\langle y \rangle$
$X_4\,(-1, +3, -1, -1)$	(14)	$\langle 122234\rangle$
$X_4\,(-1, -1, +3, -1)$	$(15)\,(24)$	$\langle 123334\rangle$
$X_4\,(-1, -1, -1, +3)$	$(16)\,(24)\,(35)$	$\langle 123444\rangle$

Tab. 31: The class $X_4\,(+1, -1, 0, 0)$: $d_4 = 36$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle\{134\}\,\{234\}\rangle$	$-\,(24)\,(35)\,\eta\vartheta$	$\langle 123344\rangle$
Derived classes	$\tilde{\pi}$	$\langle y \rangle$
$X_4\,(+1, 0, -1, 0)$	(24)	$\langle 122344\rangle$
$X_4\,(+1, 0, 0, -1)$	$(26)\,(35)$	$\langle 122334\rangle$
$X_4\,(0, +1, -1, 0)$	$(13)\,(24)$	$\langle 112344\rangle$
$X_4\,(0, +1, 0, -1)$	$(135)\,(26)$	$\langle 112334\rangle$
$X_4\,(0, 0, +1, -1)$	$(15)\,(26)$	$\langle 112234\rangle$

Tab. 32: The class $X_4\,(+2,-1,-1,0)$: $d_4 = 18$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 114\,\{234\}\rangle$	$(354)\,\vartheta$	$\langle 112344\rangle$
$\langle 141\,\{234\}\rangle$	$(2543)\,\vartheta$	
$\langle 411\,\{234\}\rangle$	$(1543)\,\vartheta$	
Derived classes	$\tilde{\pi}$	$\langle y \rangle$
$X_4\,(-1,+2,-1,0)$	(13)	$\langle 122344\rangle$
$X_4\,(+2,-1,0,-1)$	(46)	$\langle 112334\rangle$
$X_4\,(+2,0,-1,-1)$	$(36)\,(45)$	$\langle 112234\rangle$
$X_4\,(0,+2,-1,-1)$	$(145)\,(236)$	$\langle 112234\rangle$
$X_4\,(0,-1,+2,-1)$	$(15)\,(2436)$	$\langle 112334\rangle$
$X_4\,(-1,+2,0,-1)$	(1364)	$\langle 122334\rangle$
$X_4\,(-1,-1,+2,0)$	$(13)\,(24)$	$\langle 123344\rangle$
$X_4\,(-1,-1,0,+2)$	$(164)\,(253)$	$\langle 123344\rangle$
$X_4\,(-1,0,+2,-1)$	$(14)\,(25)\,(36)$	$\langle 122334\rangle$
$X_4\,(-1,0,-1,+2)$	$(1634)\,(25)$	$\langle 122344\rangle$
$X_4\,(0,-1,-1,+2)$	$(15)\,(26)$	$\langle 112344\rangle$

B.4 5–shell case

Tab. 33: The class $X_5\,(+2,+1,-1,-1,-1)$: $d_5 = 18$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle 112\,\{345\}\rangle$	ϑ	$\langle 112345\rangle$
$\langle 121\,\{345\}\rangle$	$(23)\,\vartheta$	
$\langle 211\,\{345\}\rangle$	$(13)\,\vartheta$	
Derived classes	$\tilde{\pi}$	$\langle y \rangle$
$X_5\,(+2,-1,+1,-1,-1)$	(34)	$\langle 112345\rangle$
$X_5\,(+2,-1,-1,+1,-1)$	(35)	
$X_5\,(+2,-1,-1,-1,+1)$	(36)	
$X_5\,(+1,+2,-1,-1,-1)$	(13)	$\langle 122345\rangle$
$X_5\,(-1,+2,+1,-1,-1)$	(134)	
$X_5\,(-1,+2,-1,+1,-1)$	(135)	
$X_5\,(-1,+2,-1,-1,+1)$	(136)	
$X_5\,(-1,-1,+2,+1,-1)$	$(135)\,(24)$	$\langle 123345\rangle$
$X_5\,(-1,+1,+2,-1,-1)$	$(14)\,(23)$	
$X_5\,(+1,-1,+2,-1,-1)$	$(13)\,(24)$	
$X_5\,(-1,-1,+2,-1,+1)$	$(136)\,(24)$	
$X_5\,(-1,+1,-1,+2,-1)$	$(14)\,(253)$	$\langle 123445\rangle$
$X_5\,(+1,-1,-1,+2,-1)$	$(153)\,(24)$	
$X_5\,(-1,-1,+1,+2,-1)$	$(15)\,(24)$	
$X_5\,(-1,-1,-1,+2,+1)$	$(1436)\,(25)$	
$X_5\,(+1,-1,-1,-1,+2)$	$(1543)\,(26)$	$\langle 123455\rangle$
$X_5\,(-1,-1,+1,-1,+2)$	$(16)\,(254)$	
$X_5\,(-1,+1,-1,-1,+2)$	$(154)\,(263)$	
$X_5\,(-1,-1,-1,+1,+2)$	$(15)\,(2634)$	

Tab. 34: The class $X_5\,(+1,+1,-1,-1,0)$: $d_5 = 36$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle \{125\}\,\{345\} \rangle$	$(354)\,\eta\vartheta$	$\langle 123455 \rangle$
Derived classes	$\tilde{\pi}$	$\langle y \rangle$
$X_5\,(+1,-1,+1,-1,0)$	(23)	$\langle 123455 \rangle$
$X_5\,(+1,-1,-1,+1,0)$	(24)	
$X_5\,(+1,+1,-1,0,-1)$	(46)	$\langle 123445 \rangle$
$X_5\,(+1,-1,+1,0,-1)$	$(23)\,(46)$	
$X_5\,(+1,-1,-1,0,+1)$	(264)	
$X_5\,(+1,+1,0,-1,-1)$	$(35)\,(46)$	$\langle 123345 \rangle$
$X_5\,(+1,-1,0,+1,-1)$	$(254)\,(36)$	
$X_5\,(+1,-1,0,-1,+1)$	$(263)\,(45)$	
$X_5\,(+1,0,+1,-1,-1)$	$(245)\,(36)$	$\langle 122345 \rangle$
$X_5\,(+1,0,-1,+1,-1)$	$(25)\,(346)$	
$X_5\,(+1,0,-1,-1,+1)$	$(26)\,(345)$	
$X_5\,(0,+1,+1,-1,-1)$	$(146)\,(235)$	$\langle 112345 \rangle$
$X_5\,(0,+1,-1,+1,-1)$	$(15)\,(2346)$	
$X_5\,(0,+1,-1,-1,+1)$	$(16)\,(2345)$	

B.5 6–shell case

Tab. 35: The class $X_6\,(+1,+1,+1,-1,-1,-1)$: $d_6 = 36$

$\langle x_\pi \rangle$	π	$\langle x \rangle$
$\langle \{123\}\,\{456\} \rangle$	$\eta\vartheta$	$\langle 123456 \rangle$
Derived classes	$\tilde{\pi}$	$\langle y \rangle$
$X_6\,(+1,+1,-1,+1,-1,-1)$	(34)	$\langle 123456 \rangle$
$X_6\,(+1,+1,-1,-1,+1,-1)$	(35)	
$X_6\,(+1,+1,-1,-1,-1,+1)$	(36)	
$X_6\,(+1,-1,+1,+1,-1,-1)$	(24)	
$X_6\,(+1,-1,+1,-1,+1,-1)$	(254)	
$X_6\,(+1,-1,+1,-1,-1,+1)$	(264)	
$X_6\,(+1,-1,-1,+1,+1,-1)$	$(24)\,(35)$	
$X_6\,(+1,-1,-1,+1,-1,+1)$	$(24)\,(36)$	
$X_6\,(+1,-1,-1,-1,+1,+1)$	$(25)\,(36)$	

In tables, the notation $\langle ijk\{lpq\} \rangle$ considers the set

$$\{\langle ijklpq \rangle, \langle ijklqp \rangle, \langle ijkplq \rangle, \langle ijkpql \rangle, \langle ijkqlp \rangle, \langle ijkqpl \rangle\},$$

where each of the scheme in a given set is prescribed by the corresponding permutation ϑ from the set

$$\vartheta \in \{1_6, (56), (45), (456), (465), (46)\}.$$

Similarly, the notation $\langle \{ijk\}lpq \rangle$ considers the set

$$\{\langle ijklpq \rangle, \langle ikjlpq \rangle, \langle jiklpq \rangle, \langle jkilpq \rangle, \langle kijlpq \rangle, \langle kjilpq \rangle\},$$

and each of the scheme in the set is prescribed by the corresponding permutation η from the set

$$\eta \in \{1_6, (23), (12), (123), (132), (13)\}.$$

Finally, the notation $\langle \{ijk\}\{lpq\} \rangle$ is a union of both sets.

B.6 Identification of operators associated to classes

Tab. 36: The classes for 3–shell case

$X_3(\Delta_1, \Delta_2, \Delta_3)$	$X_3^*(\Delta_1, \Delta_2, \Delta_3)$	$X_3(\Delta_1', \Delta_2', \Delta_3')$	$X_3^*(\Delta_1', \Delta_2', \Delta_3')$
$X_3(0,0,0)$	$X_3(0,0,0)$	$X_3(0,0,0)$	$X_3(0,0,0)$
$X_3(+2,-1,-1)$	$X_3(-2,+1,+1)$	$X_3(-1,+2,-1)$	$X_3(+1,-2,+1)$
		$X_3(-1,-1,+2)$	$X_3(+1,+1,-2)$
$X_3(+3,-2,-1)$	$X_3(-3,+2,+1)$	$X_3(-2,+3,-1)$	$X_3(+2,-3,+1)$
		$X_3(-1,-2,+3)$	$X_3(+1,+2,-3)$
		$X_3(+3,-1,-2)$	$X_3(-3,+1,+2)$
		$X_3(-1,+3,-2)$	$X_3(+1,-3,+2)$
		$X_3(-2,-1,+3)$	$X_3(+2,+1,-3)$
$X_3(+1,-1,0)$	$X_3(-1,+1,0)$	$X_3(+1,0,-1)$	$X_3(-1,0,+1)$
		$X_3(0,+1,-1)$	$X_3(0,-1,+1)$
$X_3(+2,-2,0)$	$X_3(-2,+2,0)$	$X_3(+2,0,-2)$	$X_3(-2,0,+2)$
		$X_3(0,+2,-2)$	$X_3(0,-2,+2)$

Tab. 37: The classes for 4–shell case

$X_4(\Delta_1, \Delta_2, \Delta_3, \Delta_4)$	$X_4^*(\Delta_1, \Delta_2, \Delta_3, \Delta_4)$	$X_4(\Delta_1', \Delta_2', \Delta_3', \Delta_4')$	$X_4^*(\Delta_1', \Delta_2', \Delta_3', \Delta_4')$
$X_4(+1,+1,-1,-1)$	$X_4(-1,-1,+1,+1)$	$X_4(+1,-1,+1,-1)$	$X_4(-1,+1,-1,+1)$
		$X_4(+1,-1,-1,+1)$	$X_4(-1,+1,+1,-1)$
$X_4(+2,-2,+1,-1)$	$X_4(-2,+2,-1,+1)$	$X_4(+2,-2,-1,+1)$	$X_4(-2,+2,+1,-1)$
		$X_4(+2,+1,-2,-1)$	$X_4(-2,-1,+2,+1)$
		$X_4(+2,+1,-1,-2)$	$X_4(-2,-1,+1,+2)$
		$X_4(+2,-1,-2,+1)$	$X_4(-2,+1,+2,-1)$
		$X_4(+2,-1,+1,-2)$	$X_4(-2,+1,-1,+2)$
		$X_4(+1,+2,-2,-1)$	$X_4(-1,-2,+2,+1)$
		$X_4(+1,+2,-1,-2)$	$X_4(-1,-2,+1,+2)$
		$X_4(+1,-2,+2,-1)$	$X_4(-1,+2,-2,+1)$
		$X_4(+1,-2,-1,+2)$	$X_4(-1,+2,+1,-2)$
		$X_4(+1,-1,+2,-2)$	$X_4(-1,+1,-2,+2)$
		$X_4(+1,-1,-2,+2)$	$X_4(-1,+1,+2,-2)$
$X_4(+3,-1,-1,-1)$	$X_4(-3,+1,+1,+1)$	$X_4(-1,+3,-1,-1)$	$X_4(+1,-3,+1,+1)$
		$X_4(-1,-1,+3,-1)$	$X_4(+1,+1,-3,+1)$
		$X_4(-1,-1,-1,+3)$	$X_4(+1,+1,+1,-3)$
$X_4(+2,-1,-1,0)$	$X_4(-2,+1,+1,0)$	$X_4(-1,+2,-1,0)$	$X_4(+1,-2,+1,0)$
		$X_4(+2,-1,0,-1)$	$X_4(-2,+1,0,+1)$
		$X_4(+2,0,-1,-1)$	$X_4(-2,0,+1,+1)$
		$X_4(0,+2,-1,-1)$	$X_4(0,-2,+1,+1)$
		$X_4(0,-1,+2,-1)$	$X_4(0,+1,-2,+1)$
		$X_4(-1,+2,0,-1)$	$X_4(+1,-2,0,+1)$
		$X_4(-1,-1,0,+2)$	$X_4(+1,+1,0,-2)$
		$X_4(-1,0,+2,-1)$	$X_4(+1,0,-2,+1)$
		$X_4(-1,0,-1,+2)$	$X_4(+1,0,+1,-2)$
		$X_4(0,-1,-1,+2)$	$X_4(0,+1,+1,-2)$
$X_4(+1,-1,0,0)$	$X_4(-1,+1,0,0)$	$X_4(+1,0,-1,0)$	$X_4(-1,0,+1,0)$
		$X_4(+1,0,0,-1)$	$X_4(-1,0,0,+1)$
		$X_4(0,+1,-1,0)$	$X_4(0,-1,+1,0)$
		$X_4(0,+1,0,-1)$	$X_4(0,-1,0,+1)$
		$X_4(0,0,+1,-1)$	$X_4(0,0,-1,+1)$

Tab. 38: The classes for 5–shell case

$X_5\,(\Delta_1, \Delta_2, \Delta_3, \Delta_4, \Delta_5)$	$X_5^*\,(\Delta_1, \Delta_2, \Delta_3, \Delta_4, \Delta_5)$	$X_5\,(\Delta_1', \Delta_2', \Delta_3', \Delta_4', \Delta_5')$	$X_5^*\,(\Delta_1', \Delta_2', \Delta_3', \Delta_4', \Delta_5')$
$X_5\,(+2,+1,-1,-1,-1)$	$X_5\,(-2,-1,+1,+1,+1)$	$X_5\,(+2,-1,+1,-1,-1)$	$X_5\,(-2,+1,-1,+1,+1)$
		$X_5\,(+2,-1,-1,+1,-1)$	$X_5\,(-2,+1,+1,-1,+1)$
		$X_5\,(+2,-1,-1,-1,+1)$	$X_5\,(-2,+1,+1,+1,-1)$
		$X_5\,(+1,+2,-1,-1,-1)$	$X_5\,(-1,-2,+1,+1,+1)$
		$X_5\,(-1,+2,+1,-1,-1)$	$X_5\,(+1,-2,-1,+1,+1)$
		$X_5\,(-1,+2,-1,+1,-1)$	$X_5\,(+1,-2,+1,-1,+1)$
		$X_5\,(-1,+2,-1,-1,+1)$	$X_5\,(+1,-2,+1,+1,-1)$
		$X_5\,(-1,-1,+2,+1,-1)$	$X_5\,(+1,+1,-2,-1,+1)$
		$X_5\,(-1,+1,+2,-1,-1)$	$X_5\,(+1,-1,-2,+1,+1)$
		$X_5\,(+1,-1,+2,-1,-1)$	$X_5\,(-1,+1,-2,+1,+1)$
		$X_5\,(-1,-1,+2,-1,+1)$	$X_5\,(+1,+1,-2,+1,-1)$
		$X_5\,(-1,+1,-1,+2,-1)$	$X_5\,(+1,-1,+1,-2,+1)$
		$X_5\,(+1,-1,-1,+2,-1)$	$X_5\,(-1,+1,+1,-2,+1)$
		$X_5\,(-1,-1,+1,+2,-1)$	$X_5\,(+1,+1,-1,-2,+1)$
		$X_5\,(-1,-1,-1,+2,+1)$	$X_5\,(+1,+1,+1,-2,-1)$
		$X_5\,(+1,-1,-1,-1,+2)$	$X_5\,(-1,+1,+1,+1,-2)$
		$X_5\,(-1,-1,+1,-1,+2)$	$X_5\,(+1,+1,-1,+1,-2)$
		$X_5\,(-1,+1,-1,-1,+2)$	$X_5\,(+1,-1,+1,+1,-2)$
		$X_5\,(-1,-1,-1,+1,+2)$	$X_5\,(+1,+1,+1,-1,-2)$
$X_5\,(+1,+1,-1,-1,0)$	$X_5\,(-1,-1,+1,+1,0)$	$X_5\,(+1,-1,+1,-1,0)$	$X_5\,(-1,+1,-1,+1,0)$
		$X_5\,(+1,-1,-1,+1,0)$	$X_5\,(-1,+1,+1,-1,0)$
		$X_5\,(+1,+1,-1,0,-1)$	$X_5\,(-1,-1,+1,0,+1)$
		$X_5\,(+1,-1,+1,0,-1)$	$X_5\,(-1,+1,-1,0,+1)$
		$X_5\,(+1,-1,-1,0,+1)$	$X_5\,(-1,+1,+1,0,-1)$
		$X_5\,(+1,+1,0,-1,-1)$	$X_5\,(-1,-1,0,+1,+1)$
		$X_5\,(+1,-1,0,+1,-1)$	$X_5\,(-1,+1,0,-1,+1)$
		$X_5\,(+1,-1,0,-1,+1)$	$X_5\,(-1,+1,0,+1,-1)$
		$X_5\,(+1,0,+1,-1,-1)$	$X_5\,(-1,0,-1,+1,+1)$
		$X_5\,(+1,0,-1,+1,-1)$	$X_5\,(-1,0,+1,-1,+1)$
		$X_5\,(+1,0,-1,-1,+1)$	$X_5\,(-1,0,+1,+1,-1)$
		$X_5\,(0,+1,+1,-1,-1)$	$X_5\,(0,-1,-1,+1,+1)$
		$X_5\,(0,+1,-1,+1,-1)$	$X_5\,(0,-1,+1,-1,+1)$
		$X_5\,(0,+1,-1,-1,+1)$	$X_5\,(0,-1,+1,+1,-1)$

Tab. 39: The classes for 6–shell case

$X_6\,(\Delta_1, \Delta_2, \Delta_3, \Delta_4, \Delta_5, \Delta_6)$	$X_6^*\,(\Delta_1, \Delta_2, \Delta_3, \Delta_4, \Delta_5, \Delta_6)$	$X_6\,(\Delta_1', \Delta_2', \Delta_3', \Delta_4', \Delta_5', \Delta_6')$	$X_6^*\,(\Delta_1', \Delta_2', \Delta_3', \Delta_4', \Delta_5', \Delta_6')$
$X_6\,(+1,+1,+1,-1,-1,-1)$	$X_6\,(-1,-1,-1,+1,+1,+1)$	$X_6\,(+1,+1,-1,+1,-1,-1)$	$X_6\,(-1,-1,+1,-1,+1,+1)$
		$X_6\,(+1,+1,-1,-1,+1,-1)$	$X_6\,(-1,-1,+1,+1,-1,+1)$
		$X_6\,(+1,+1,-1,-1,-1,+1)$	$X_6\,(-1,-1,+1,+1,+1,-1)$
		$X_6\,(+1,-1,+1,+1,-1,-1)$	$X_6\,(-1,+1,-1,-1,+1,+1)$
		$X_6\,(+1,-1,+1,-1,+1,-1)$	$X_6\,(-1,+1,-1,+1,-1,+1)$
		$X_6\,(+1,-1,+1,-1,-1,+1)$	$X_6\,(-1,+1,-1,+1,+1,-1)$
		$X_6\,(+1,-1,-1,+1,+1,-1)$	$X_6\,(-1,+1,+1,-1,-1,+1)$
		$X_6\,(+1,-1,-1,+1,-1,+1)$	$X_6\,(-1,+1,+1,-1,+1,-1)$
		$X_6\,(+1,-1,-1,-1,+1,+1)$	$X_6\,(-1,+1,+1,+1,-1,-1)$

C SU(2)–invariant part of the second-order wave operator

C.1 One-body part

$$\begin{aligned}&\Omega^{(2)+}_{\mu\mathrm{c}}(\Lambda)(\varepsilon_{\mathrm{c}}-\varepsilon_{\mu})=\delta_{\Lambda\tau}[\ddot{S}_{\mu\mathrm{c}}(\tau_1\tau_2\tau)+\dot{S}_{\mu\mathrm{c}}(\tau_1\tau_2\tau)]+\delta_{\Lambda\tau_1}[\widetilde{\ddot{S}}_{\mu\mathrm{c}}(\tau_1)+\widetilde{\dot{S}}_{\mu\mathrm{c}}(\tau_1)]\\&+\delta_{\Lambda\tau_2}[\widetilde{\ddot{S}}'_{\mu\mathrm{c}}(\tau_2)+\widetilde{\dot{S}}'_{\mu\mathrm{c}}(\tau_2)]+\delta_{\Lambda 0}\widetilde{S}_{\mu\mathrm{c}},\end{aligned}\tag{C.1a}$$

$$\Omega^{(2)-}_{\mu\mathrm{c}}(\Lambda)(\varepsilon_{\mathrm{c}}-\varepsilon_{\mu})=\delta_{\Lambda\tau}S_{\mathrm{c}\mu}(\tau_1\tau_2\tau).\tag{C.1b}$$

$$\begin{aligned}&\Omega^{(2)+}_{\mathrm{ev}}(\Lambda)(\varepsilon_{\mathrm{v}}-\varepsilon_{\mathrm{e}})=\delta_{\Lambda\tau}\ddot{S}_{\mathrm{ev}}(\tau_1\tau_2\tau)+\delta_{\Lambda\tau_1}[\widetilde{\ddot{S}}_{\mathrm{ev}}(\tau_1)+\widetilde{\dot{S}}_{\mathrm{ev}}(\tau_1)]\\&+\delta_{\Lambda\tau_2}[\widetilde{\ddot{S}}'_{\mathrm{ev}}(\tau_2)+\widetilde{\dot{S}}'_{\mathrm{ev}}(\tau_2)]+\delta_{\Lambda 0}\widetilde{S}_{\mathrm{ev}},\end{aligned}\tag{C.2a}$$

$$\Omega^{(2)-}_{\mathrm{ev}}(\Lambda)(\varepsilon_{\mathrm{v}}-\varepsilon_{\mathrm{e}})=\delta_{\Lambda\tau}[\dot{S}_{\mathrm{ve}}(\tau_1\tau_2\tau)+\ddot{S}_{\mathrm{ve}}(\tau_1\tau_2\tau)].\tag{C.2b}$$

C.2 Two-body part

$$\begin{aligned}&\Omega^{(2)+}_{\mu\mu'\mathrm{cc}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{cc}'}-\varepsilon_{\mu\mu'})\\&=\delta_{\Lambda_1 u}\delta_{\Lambda_2 d}\delta_{\Lambda\tau}D_{\mu\mu'\mathrm{cc}'}(ud\tau)+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}[\mathfrak{X}_{\mu\mu'\mathrm{cc}'}(Uu\tau_1)+\tfrac{1}{2}\widetilde{\mathfrak{Y}}_{\mu\mu'\mathrm{cc}'}(Uu\tau_1)]\\&+\tfrac{1}{2}\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\mathcal{Z}_{\mu'\mu\mathrm{cc}'}(Uu\tau_2)\widetilde{D'}_{\mu'\mu\mathrm{cc}'}(Uu\tau_2)-\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}[\tfrac{1}{4}\ddot{D}_{\mu\mu'\mathrm{cc}'}(\widetilde{u}u)\\&+\tfrac{1}{4}\dot{D}_{\mu\mu'\mathrm{cc}'}(\widetilde{u}u)+\tfrac{1}{2}\ddot{\mathfrak{Z}}_{\mu\mu'\mathrm{cc}'}(\widetilde{u}u)+\dot{\Delta}_{\mu\mu'\mathrm{cc}'}(uu)+\ddot{\Delta}_{\mu\mu'\mathrm{cc}'}(uu)],\end{aligned}\tag{C.3a}$$

$$\begin{aligned}&\Omega^{(2)-}_{\mu\mu'\mathrm{cc}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{cc}'}-\varepsilon_{\mu\mu'})\\&=-\tfrac{1}{2}\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}\mathcal{Z}_{\mathrm{c}'\mathrm{c}\mu\mu'}(uU\tau_1)\widetilde{D}_{\mathrm{c}'\mathrm{c}\mu\mu'}(uU\tau_1)+\tfrac{1}{2}\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\mathcal{Z}_{\mathrm{c}'\mathrm{c}\mu\mu'}(uU\tau_2)\\&\times[\widetilde{\ddot{D}'}_{\mathrm{c}'\mathrm{c}\mu\mu'}(uU\tau_2)+\widetilde{\dot{D}'}_{\mathrm{c}'\mathrm{c}\mu\mu'}(uU\tau_2)]+\tfrac{1}{4}\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}\mathcal{Z}_{\mathrm{cc}'\mu\mu'}(u)D_{\mathrm{cc}'\mu\mu'}(u\widetilde{u}).\end{aligned}\tag{C.3b}$$

$$\begin{aligned}&\Omega^{(2)+}_{\mathrm{evcc}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{cc}'}-\varepsilon_{\mathrm{ev}})\\&=-\delta_{\Lambda_1 u}\delta_{\Lambda_2 d}\delta_{\Lambda\tau}\mathcal{Z}_{\mathrm{vecc}'}(ud\tau)D_{\mathrm{vecc}'}(ud\tau)+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}[\ddot{D}_{\mathrm{evcc}'}(Uu\tau_1)\\&+\mathcal{Z}_{\mathrm{vec}'\mathrm{c}}(Uu\tau_1)\dot{D}_{\mathrm{vec}'\mathrm{c}}(Uu\tau_1)+\tfrac{1}{2}\widetilde{\dot{D}}_{\mathrm{evcc}'}(Uu\tau_1)-\tfrac{1}{2}\mathcal{Z}_{\mathrm{vecc}'}(Uu\tau_1)\widetilde{\ddot{D}}_{\mathrm{vecc}'}(Uu\tau_1)]\\&+\tfrac{1}{2}\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}[-\widetilde{D'}_{\mathrm{evcc}'}(Uu\tau_2)+\mathcal{Z}_{\mathrm{vecc}'}(Uu\tau_2)\widetilde{D'}_{\mathrm{vecc}'}(Uu\tau_2)]-\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}\\&\times[\widetilde{\ddot{\Delta}}_{\mathrm{evcc}'}(uu)+\widetilde{\dot{\Delta}}_{\mathrm{evcc}'}(uu)-\mathcal{Z}_{\mathrm{vecc}'}(u)\{\widetilde{\ddot{\Delta}}_{\mathrm{vecc}'}(uu)+\widetilde{\dot{\Delta}}_{\mathrm{vecc}'}(uu)\}\\&+\mathcal{Z}_{\mathrm{evc}'\mathrm{c}}(u)\ddot{D}_{\mathrm{evc}'\mathrm{c}}(u\widetilde{u})],\end{aligned}\tag{C.4a}$$

$$\begin{aligned}&\Omega^{(2)-}_{\mathrm{evcc}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{cc}'}-\varepsilon_{\mathrm{ev}})\\&=-\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}\mathcal{Z}_{\mathrm{c}'\mathrm{cev}}(uU\tau_1)\widetilde{D}_{\mathrm{c}'\mathrm{cev}}(uU\tau_1)+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\mathcal{Z}_{\mathrm{c}'\mathrm{cev}}(uU\tau_2)\\&\times[\widetilde{\ddot{D}'}_{\mathrm{c}'\mathrm{cev}}(uU\tau_2)+\widetilde{\dot{D}'}_{\mathrm{c}'\mathrm{cev}}(uU\tau_2)].\end{aligned}\tag{C.4b}$$

$$\begin{aligned}&\Omega^{(2)+}_{\mu\mu'\mathrm{c}\bar{\mathrm{v}}}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{c}\bar{\mathrm{v}}}-\varepsilon_{\mu\mu'})\\&=\delta_{\Lambda_1 u}\delta_{\Lambda_2 d}\delta_{\Lambda\tau}\delta_{\mu\mathrm{e}}[D_{\mathrm{ee}'\mathrm{c}\bar{\mathrm{v}}}(ud\tau)-\mathcal{Z}_{\mathrm{ee}'\bar{\mathrm{v}}\mathrm{c}}(ud\tau)D_{\mathrm{ee}'\bar{\mathrm{v}}\mathrm{c}}(ud\tau)]+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}\\&\times[\widetilde{\ddot{D}}_{\mu\mu'\mathrm{c}\bar{\mathrm{v}}}(Uu\tau_1)-\mathcal{Z}_{\mu\mu'\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_1)\widetilde{\dot{D}}_{\mu\mu'\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_1)]+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\mathcal{Z}_{\mu'\mu\mathrm{c}\bar{\mathrm{v}}}(Uu\tau_2)\\&\times\widetilde{D'}_{\mu'\mu\mathrm{c}\bar{\mathrm{v}}}(Uu\tau_2)+\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}[\mathcal{Z}_{\mu\mu'\bar{\mathrm{v}}\mathrm{c}}(u)\{\widetilde{\ddot{\Delta}}_{\mu\mu'\bar{\mathrm{v}}\mathrm{c}}(uu)+\widetilde{\dot{\Delta}}_{\mu\mu'\bar{\mathrm{v}}\mathrm{c}}(uu)\}\\&-\widetilde{\ddot{\Delta}}_{\mu\mu'\mathrm{c}\bar{\mathrm{v}}}(uu)-\widetilde{\dot{\Delta}}_{\mu\mu'\mathrm{c}\bar{\mathrm{v}}}(uu)-\tfrac{1}{2}\widetilde{\ddot{D}}_{\mu\mu'\mathrm{c}\bar{\mathrm{v}}}(uu)],\end{aligned}\tag{C.5a}$$

$$\begin{aligned}&\Omega^{(2)-}_{\mu\mu'\mathrm{c}\bar{\mathrm{v}}}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{c}\bar{\mathrm{v}}}-\varepsilon_{\mu\mu'})\\&=-\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}[\mathcal{Z}_{\bar{\mathrm{v}}\mathrm{c}\mu\mu'}(uU\tau_1)\{\dot{D}_{\bar{\mathrm{v}}\mathrm{c}\mu\mu'}(uU\tau_1)+\tfrac{1}{2}\widetilde{D}_{\bar{\mathrm{v}}\mathrm{c}\mu\mu'}(uU\tau_1)\}+\mathcal{Z}_{\mathrm{c}\bar{\mathrm{v}}\mu'\mu}(uU\tau_1)\\&\times D_{\mathrm{c}\bar{\mathrm{v}}\mu'\mu}(uU\tau_1)]-\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}[\mathcal{Z}_{\mathrm{c}\bar{\mathrm{v}}\mu\mu'}(uU\tau_2)\{\widetilde{\ddot{D}'}_{\mathrm{c}\bar{\mathrm{v}}\mu\mu'}(uU\tau_2)+\widetilde{\dot{D}'}_{\mathrm{c}\bar{\mathrm{v}}\mu\mu'}(uU\tau_2)\}\\&-\mathcal{Z}_{\bar{\mathrm{v}}\mathrm{c}\mu\mu'}(uU\tau_2)\widetilde{\ddot{D}'}_{\bar{\mathrm{v}}\mathrm{c}\mu\mu'}(uU\tau_2)].\end{aligned}\tag{C.5b}$$

$$\begin{aligned}
&\Omega^{(2)+}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{c}\bar{\mathrm{v}}}-\varepsilon_{\mathrm{ev}})\\
&=\delta_{\Lambda_1 u}\delta_{\Lambda_2 d}\delta_{\Lambda\tau}[D_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(ud\tau)+\mathcal{Z}_{\mathrm{vec}\bar{\mathrm{v}}}(ud\tau)D_{\mathrm{vec}\bar{\mathrm{v}}}(ud\tau)]+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}[\widetilde{\ddot{D}}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_1)\\
&+\widetilde{\dot{D}}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_1)-\mathcal{Z}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_1)\{\widetilde{\ddot{D}}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_1)+\widetilde{\dot{D}}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_1)\}]+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\\
&\times[-\widetilde{D'}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_2)+\mathcal{Z}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_2)\widetilde{D'}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(Uu\tau_2)]-\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}[\widetilde{\ddot{\Delta}}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(uu)\\
&+\widetilde{\dot{\Delta}}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(uu)+\widetilde{\ddot{D}}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(uu)-\mathcal{Z}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(u)\{\widetilde{\ddot{\Delta}}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(uu)+\widetilde{\dot{\Delta}}_{\mathrm{ve}\bar{\mathrm{v}}\mathrm{c}}(uu)\}-\mathcal{Z}_{\mathrm{evc}\bar{\mathrm{v}}}(u)\\
&\times\{\widetilde{\ddot{\Delta}}_{\mathrm{evc}\bar{\mathrm{v}}}(uu)+\widetilde{\dot{\Delta}}_{\mathrm{evc}\bar{\mathrm{v}}}(uu)\}+\mathcal{Z}_{\mathrm{vec}\bar{\mathrm{v}}}(u)\{\widetilde{\ddot{\Delta}}_{\mathrm{vec}\bar{\mathrm{v}}}(uu)+\widetilde{\dot{\Delta}}_{\mathrm{vec}\bar{\mathrm{v}}}(uu)\}],
\end{aligned}\tag{C.6a}$$

$$\begin{aligned}
&\Omega^{(2)-}_{\mathrm{ev}\bar{\mathrm{v}}\mathrm{c}}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\mathrm{c}\bar{\mathrm{v}}}-\varepsilon_{\mathrm{ev}})\\
&=\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}[\mathcal{Z}_{\bar{\mathrm{v}}\mathrm{cev}}(uU\tau_1)\{\widetilde{D}_{\bar{\mathrm{v}}\mathrm{cev}}(uU\tau_1)-\widetilde{\dot{D}}_{\bar{\mathrm{v}}\mathrm{cev}}(uU\tau_1)\}-\mathcal{Z}_{\mathrm{c}\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_1)\\
&\times\widetilde{D}_{\mathrm{c}\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_1)]+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}[-\mathcal{Z}_{\bar{\mathrm{v}}\mathrm{cev}}(uU\tau_2)\widetilde{\ddot{D}'}_{\bar{\mathrm{v}}\mathrm{cev}}(uU\tau_2)+\mathcal{Z}_{\mathrm{c}\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_2)\\
&\times\{\widetilde{\ddot{D}'}_{\mathrm{c}\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_2)-\widetilde{\dot{D}'}_{\mathrm{c}\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_2)\}].
\end{aligned}\tag{C.6b}$$

$$\begin{aligned}
&\Omega^{(2)+}_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'}-\varepsilon_{\mathrm{ev}})\\
&=\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}[\ddot{D}_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_1)+\mathcal{Z}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_1)\{\dot{D}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_1)-\tfrac{1}{2}\widetilde{\ddot{D}}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_1)\}]\\
&+\tfrac{1}{2}\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}[\mathcal{Z}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_2)\widetilde{D'}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_2)-\widetilde{D'}_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_2)-\dot{D}'_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_2)]\\
&+\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}[-\widetilde{\ddot{\Delta}}_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(uu)-\widetilde{\dot{\Delta}}_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(uu)+\mathcal{Z}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(u)\{\widetilde{\ddot{\Delta}}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(uu)+\widetilde{\dot{\Delta}}_{\mathrm{ve}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(uu)\}],
\end{aligned}\tag{C.7a}$$

$$\begin{aligned}
&\Omega^{(2)-}_{\mathrm{ev}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'}-\varepsilon_{\mathrm{ev}})\\
&=-\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}\mathcal{Z}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_1)[\widetilde{D}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_1)+\widetilde{\dot{D}}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_1)]+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\\
&\times\mathcal{Z}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_2)\widetilde{\ddot{D}}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ev}}(uU\tau_2)-\tfrac{1}{2}\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}\mathcal{Z}_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{ev}}(u)\dot{D}_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{ev}}(u\widetilde{u}).
\end{aligned}\tag{C.7b}$$

$$\begin{aligned}
&\Omega^{(2)+}_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'}-\varepsilon_{\mathrm{ee}'})\\
&=\delta_{\Lambda_1 u}\delta_{\Lambda_2 d}\delta_{\Lambda\tau}D_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(ud\tau)+\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}[\tfrac{1}{2}\widetilde{\ddot{D}}_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_1)+\dot{D}_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_1)]\\
&+\tfrac{1}{2}\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\mathcal{Z}_{\mathrm{e}'\mathrm{e}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_2)\widetilde{D'}_{\mathrm{e}'\mathrm{e}\bar{\mathrm{v}}\bar{\mathrm{v}}'}(Uu\tau_2)-\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}[\tfrac{1}{2}\{\tfrac{1}{2}\ddot{D}_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(\widetilde{u}u)\\
&-\mathcal{Z}_{\mathrm{ee}'\bar{\mathrm{v}}'\bar{\mathrm{v}}}(u)\dddot{D}_{\mathrm{ee}'\bar{\mathrm{v}}'\bar{\mathrm{v}}}(\widetilde{u}u)\}+\widetilde{\ddot{\Delta}}_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(uu)+\widetilde{\dot{\Delta}}_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(uu)],
\end{aligned}\tag{C.8a}$$

$$\begin{aligned}
&\Omega^{(2)-}_{\mathrm{ee}'\bar{\mathrm{v}}\bar{\mathrm{v}}'}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'}-\varepsilon_{\mathrm{ee}'})\\
&=-\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_1}\mathcal{Z}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ee}'}(uU\tau_1)[D_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ee}'}(uU\tau_1)+\widetilde{\dot{D}}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ee}'}(uU\tau_1)]+\tfrac{1}{2}\delta_{\Lambda_1 U}\delta_{\Lambda_2 u}\delta_{\Lambda\tau_2}\\
&\times\mathcal{Z}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ee}'}(uU\tau_2)\widetilde{\ddot{D}'}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{ee}'}(uU\tau_2)+\tfrac{1}{4}\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_1 u}\delta_{\Lambda 0}\mathcal{Z}_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{ee}'}(u)[D_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{ee}'}(u\widetilde{u})\\
&-\dot{D}_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{ee}'}(u\widetilde{u})].
\end{aligned}\tag{C.8b}$$

In Eq. (C.3a), the quantities $\mathfrak{X}_{\mu\mu'\mathrm{cc}'}$, $\mathfrak{Y}_{\mu\mu'\mathrm{cc}'}$, $\mathfrak{Z}_{\mu\mu'\mathrm{cc}'}$ differ for distinct one-electron orbitals $\mu=\mathrm{v},\mathrm{e}$. If $\mu=\mathrm{v}$, then $\mathfrak{X}_{\mathrm{vv}'\mathrm{cc}'}\equiv\ddot{D}_{\mathrm{vv}'\mathrm{cc}'}$, $\mathfrak{Y}_{\mathrm{vv}'\mathrm{cc}'}\equiv\dot{D}_{\mathrm{vv}'\mathrm{cc}'}$ and $\mathfrak{Z}_{\mathrm{vv}'\mathrm{cc}'}\equiv-\mathcal{Z}_{\mathrm{vv}'\mathrm{c}'\mathrm{c}}(u)D_{\mathrm{vv}'\mathrm{c}'\mathrm{c}}$; if $\mu=\mathrm{e}$, then $\mathfrak{X}_{\mathrm{ee}'\mathrm{cc}'}\equiv\dot{D}_{\mathrm{ee}'\mathrm{cc}'}$, $\mathfrak{Y}_{\mathrm{ee}'\mathrm{cc}'}\equiv\ddot{D}_{\mathrm{ee}'\mathrm{cc}'}$, $\mathfrak{Z}_{\mathrm{ee}'\mathrm{cc}'}\equiv D_{\mathrm{ee}'\mathrm{cc}'}$.

C.3 Three-body part

$$\begin{aligned}
&\Omega^{(2)+}_{\mathrm{vv}'\mathrm{v}''\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}-\varepsilon_{\mathrm{vv}'\mathrm{v}''})\\
&=\tfrac{1}{2}\delta_{\Lambda\Lambda_3}\delta_{MM_3}[\ddot{T}_{\mathrm{vv}'\mathrm{v}''\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}(\widetilde{\Lambda}_1\Lambda_2\Lambda)+\tfrac{1}{2}\widetilde{\dot{T}}_{\mathrm{vv}'\mathrm{v}''\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}(\Lambda_1\Lambda_2\Lambda)-\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}J_{\mathrm{vc}\bar{\mathrm{v}}\mathrm{c}'}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\\
&\times\{\widetilde{\ddot{T}}_{\mathrm{vv}'\mathrm{v}''\mathrm{c}'\bar{\mathrm{v}}\mathrm{c}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})+\widetilde{\dot{T}}_{\mathrm{vv}'\mathrm{v}''\mathrm{c}'\bar{\mathrm{v}}\mathrm{c}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})\}]+(-1)^{\lambda_{\mathrm{v}}+\lambda_{\mathrm{c}'}}Y_{\mathrm{vc}\bar{\mathrm{v}}\mathrm{c}'}(\Lambda_1\Lambda_2\Lambda\Lambda_3\tau_1)\\
&\times T_{\mathrm{vv}'\mathrm{v}''\mathrm{c}'\mathrm{c}\bar{\mathrm{v}}}(\Lambda_1\tau_1)+\tfrac{1}{2}\textstyle\sum_u a(\lambda_{\mathrm{v}'}\lambda_{\bar{\mathrm{v}}}u)I_{\mathrm{vv}'\mathrm{v}''\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}(\Lambda_1\Lambda_2\Lambda_3\tau_1\Lambda u)\widetilde{T}'_{\mathrm{v}''\mathrm{vv}'\mathrm{c}\bar{\mathrm{v}}\mathrm{c}'}(u\tau_2),
\end{aligned}\tag{C.9a}$$

$$\begin{aligned}
&\Omega^{(2)-}_{\mathrm{vv}'\mathrm{v}''\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}-\varepsilon_{\mathrm{vv}'\mathrm{v}''})\\
&=\tfrac{1}{2}\delta_{\Lambda\Lambda_3}\delta_{MM_3}a(\lambda_{\mathrm{v}'}\lambda_{\mathrm{v}''}\Lambda_1)[a(\lambda_{\mathrm{c}}\lambda_{\mathrm{c}'}\Lambda_2)\widetilde{T}_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{cvv}'\mathrm{v}''}(\Lambda_2\Lambda_1\Lambda)+\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}a(\lambda_{\mathrm{c}}\lambda_{\mathrm{c}'}\overline{\Lambda}_2)\\
&\times J_{\mathrm{vc}'\bar{\mathrm{v}}\mathrm{c}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)T_{\mathrm{cc}'\bar{\mathrm{v}}\mathrm{vv}'\mathrm{v}''}(\widetilde{\overline{\Lambda}}_2\Lambda_1\overline{\Lambda})].
\end{aligned}\tag{C.9b}$$

$$
\begin{aligned}
&\Omega^{(2)+}_{\mathrm{vv'e\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}-\varepsilon_{\mathrm{vv'e}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}[\tfrac{1}{2}\{-a(\lambda_{\mathrm{c}}\lambda_{\mathrm{c}'}\Lambda_2)\dot{T}_{\mathrm{vv'e\bar{v}cc'}}(\widetilde{\Lambda}_1\Lambda_2\Lambda)+\tfrac{1}{2}\widetilde{\ddot{T}}_{\mathrm{vv'e\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda)\}\\
&-a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}'}\Lambda_1)\{\ddot{T}_{\mathrm{vev'\bar{v}c'c}}(\widetilde{\Lambda}_1\Lambda_2\Lambda)+\tfrac{1}{2}\widetilde{\dot{T}}_{\mathrm{vev'\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda)\}-\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}J_{\mathrm{vc\bar{v}c'}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\\
&\times\{\tfrac{1}{2}(\widetilde{\dot{T}}_{\mathrm{vv'ec'\bar{v}c}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})+\widetilde{\ddot{T}}_{\mathrm{vv'ec'\bar{v}c}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda}))+a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}'}\Lambda_1)a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}\overline{\Lambda}_2)\\
&\times(\widetilde{\dot{T}}_{\mathrm{vev'c'c\bar{v}}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})+\widetilde{\ddot{T}}_{\mathrm{vev'c'c\bar{v}}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda}))\}]+(-1)^{\lambda_{\mathrm{v}}+\lambda_{\mathrm{c}'}}Y_{\mathrm{vc\bar{v}c'}}(\Lambda_1\Lambda_2\Lambda\Lambda_3\tau_1)\\
&\times\widetilde{T}_{\mathrm{vv'ec'c\bar{v}}}(\Lambda_1\tau_1)+\tfrac{1}{2}a(\lambda_{\mathrm{e}}\lambda_{\bar{\mathrm{v}}}\Lambda_2)Y'_{\mathrm{vv'e\bar{v}}}(\tau_1\Lambda_1\Lambda\Lambda_3\Lambda_2)T_{\mathrm{evv'\bar{v}c'c}}(\Lambda_2\tau_1)\\
&+\textstyle\sum_u[a(\lambda_{\mathrm{c}}\lambda_{\mathrm{v}'}\Lambda_2)I_{\mathrm{vv'e\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_1\Lambda u)T_{\mathrm{evv'c'c\bar{v}}}(u\tau_1)+\tfrac{1}{2}a(\lambda_{\mathrm{v}'}\lambda_{\bar{\mathrm{v}}}u)\\
&\times I_{\mathrm{vv'e\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\widetilde{T}'_{\mathrm{evv'c\bar{v}c'}}(u\tau_2)+(-1)^{\lambda_{\mathrm{v}}-\lambda_{\bar{\mathrm{v}}}}a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}'}\Lambda_1)\\
&\times I_{\mathrm{vev'\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\widetilde{T}'_{\mathrm{v'evc\bar{v}c'}}(u\tau_2)],
\end{aligned}
\tag{C.10a}
$$

$$
\begin{aligned}
&\Omega^{(2)-}_{\mathrm{vv'e\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}-\varepsilon_{\mathrm{vv'e}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}'}\Lambda_1)[a(\lambda_{\mathrm{c}}\lambda_{\mathrm{c}'}\Lambda_2)\widetilde{T}_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{cvv'e}}(\Lambda_2\Lambda_1\Lambda)\\
&+\tfrac{1}{2}\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}\{J_{\mathrm{vc\bar{v}c'}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\widetilde{T}_{\mathrm{c'c\bar{v}vv'e}}(\overline{\Lambda}_2\Lambda_1\overline{\Lambda})+(-1)^{\lambda_{\mathrm{v}}-\lambda_{\mathrm{e}}}\\
&\times\textstyle\sum_{\overline{\Lambda}_1}I'_{\mathrm{vv'e\bar{v}c'c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_1\Lambda_2\overline{\Lambda}\Lambda)(T_{\mathrm{c'c\bar{v}evv'}}(\widetilde{\overline{\Lambda}}_2\overline{\Lambda}_1\overline{\Lambda})-a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}\overline{\Lambda}_2)\\
&\times\widetilde{T}_{\mathrm{c'\bar{v}cevv'}}(\overline{\Lambda}_2\overline{\Lambda}_1\overline{\Lambda}))\}].
\end{aligned}
\tag{C.10b}
$$

$$
\begin{aligned}
&\Omega^{(2)+}_{\mathrm{ee'v\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}-\varepsilon_{\mathrm{ee'v}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}[\tfrac{1}{2}\{\ddot{T}_{\mathrm{ee'v\bar{v}c'c}}(\widetilde{\Lambda}_1\Lambda_2\Lambda)+\tfrac{1}{2}\widetilde{\dot{T}}_{\mathrm{ee'v\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda)\}+a(\lambda_{\mathrm{v}}\lambda_{\mathrm{e}'}\Lambda_1)\{a(\lambda_{\mathrm{c}}\lambda_{\mathrm{c}'}\Lambda_2)\\
&\times\dot{T}_{\mathrm{eve'\bar{v}cc'}}(\widetilde{\Lambda}_1\Lambda_2\Lambda)-\tfrac{1}{2}\widetilde{\ddot{T}}_{\mathrm{eve'\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda)\}+\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}J_{\mathrm{ec\bar{v}c'}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\\
&\times\{\tfrac{1}{2}(a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}\overline{\Lambda}_2)\widetilde{\ddot{T}}_{\mathrm{ee'vc'c\bar{v}}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})-\widetilde{\dot{T}}_{\mathrm{ee'vc'\bar{v}c}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda}))+a(\lambda_{\mathrm{v}}\lambda_{\mathrm{e}'}\Lambda_1)\\
&\times(\widetilde{\ddot{T}}_{\mathrm{eve'c'\bar{v}c}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})+\widetilde{\dot{T}}_{\mathrm{eve'c'\bar{v}c}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda}))\}]+\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_3\tau_1}\delta_{\Lambda 0}T_{\mathrm{ee'v\bar{v}c'c}}(\Lambda_1\tau_1)\\
&+(-1)^{\lambda_{\mathrm{e}}+\lambda_{\mathrm{c}'}}Y_{\mathrm{ec\bar{v}c'}}(\Lambda_1\Lambda_2\Lambda\Lambda_3\tau_1)\widetilde{T}_{\mathrm{ee'vc'c\bar{v}}}(\Lambda_1\tau_1)+\textstyle\sum_u[a(\lambda_{\mathrm{e}'}\lambda_{\mathrm{c}'}\Lambda_2)\\
&\times I_{\mathrm{ee'v\bar{v}cc'}}(\Lambda_1\Lambda_2\Lambda_3\tau_1\Lambda u)T_{\mathrm{vee'c'c\bar{v}}}(u\tau_1)+a(\lambda_{\mathrm{e}'}\lambda_{\bar{\mathrm{v}}}u)\{\tfrac{1}{2}I_{\mathrm{ee'v\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\\
&\times\widetilde{T}'_{\mathrm{vee'c\bar{v}c'}}(u\tau_2)+(-1)^{\lambda_{\mathrm{e}}-\lambda_{\mathrm{v}}}I_{\mathrm{eve'\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\widetilde{T}'_{\mathrm{e'vec\bar{v}c'}}(u\tau_2)\}],
\end{aligned}
\tag{C.11a}
$$

$$
\begin{aligned}
&\Omega^{(2)-}_{\mathrm{ee'v\bar{v}c'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{c}}-\varepsilon_{\mathrm{ee'v}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}a(\lambda_{\mathrm{v}}\lambda_{\mathrm{e}'}\Lambda_1)[a(\lambda_{\mathrm{c}}\lambda_{\mathrm{c}'}\Lambda_2)\widetilde{T}_{\bar{\mathrm{v}}\mathrm{c}'\mathrm{cee'v}}(\Lambda_2\Lambda_1\Lambda)\\
&+\tfrac{1}{2}\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}\{J_{\mathrm{ec\bar{v}c'}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\widetilde{T}_{\mathrm{c'c\bar{v}ee'v}}(\overline{\Lambda}_2\Lambda_1\overline{\Lambda})+(-1)^{\lambda_{\mathrm{e}}-\lambda_{\mathrm{v}}}\\
&\times\textstyle\sum_{\overline{\Lambda}_1}I'_{\mathrm{ee'v\bar{v}c'c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_1\Lambda_2\overline{\Lambda}\Lambda)(T_{\mathrm{c'c\bar{v}vee'}}(\widetilde{\overline{\Lambda}}_2\overline{\Lambda}_1\overline{\Lambda})-a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}\overline{\Lambda}_2)\widetilde{T}_{\mathrm{c'\bar{v}cvee'}}(\overline{\Lambda}_2\overline{\Lambda}_1\overline{\Lambda}))\}].
\end{aligned}
\tag{C.11b}
$$

$$
\begin{aligned}
&\Omega^{(2)+}_{\mathrm{vv'v''\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{c}}-\varepsilon_{\mathrm{vv'v''}})\\
&=\tfrac{1}{2}\delta_{\Lambda\Lambda_3}\delta_{MM_3}[\widetilde{\ddot{T}}_{\mathrm{vv'v''\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)+\widetilde{\dot{T}}_{\mathrm{vv'v''\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)+a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)\\
&\times\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}J_{\mathrm{v\bar{v}'\bar{v}c}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\ddot{T}_{\mathrm{vv'v''c\bar{v}\bar{v}'}}(\widetilde{\Lambda}_1\overline{\Lambda}_2\overline{\Lambda})],
\end{aligned}
\tag{C.12a}
$$

$$
\begin{aligned}
&\Omega^{(2)-}_{\mathrm{vv'v''\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{c}}-\varepsilon_{\mathrm{vv'v''}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}a(\lambda_{\mathrm{v}'}\lambda_{\mathrm{v}''}\Lambda_2)[\tfrac{1}{4}a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}'}\Lambda_1)\widetilde{T}_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{cvv'v''}}(\Lambda_2\Lambda_1\Lambda)-T_{\bar{\mathrm{v}}\mathrm{c}\bar{\mathrm{v}}'\mathrm{vv'v''}}(\widetilde{\Lambda}_2\Lambda_1\Lambda)].
\end{aligned}
\tag{C.12b}
$$

$$
\begin{aligned}
&\Omega^{(2)+}_{\mathrm{vv'e\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{c}}-\varepsilon_{\mathrm{vv'e}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}[\tfrac{1}{2}\{\widetilde{\ddot{T}}_{\mathrm{vv'e\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)+\widetilde{\dot{T}}_{\mathrm{vv'e\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)\}-a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}'}\Lambda_1)\\
&\times\{\widetilde{\ddot{T}}_{\mathrm{vev'\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)+\widetilde{\dot{T}}_{\mathrm{vev'\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)\}+a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}J_{\mathrm{v\bar{v}'\bar{v}c}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\\
&\times\{\tfrac{1}{4}\widetilde{\ddot{T}}_{\mathrm{vv'ec\bar{v}\bar{v}'}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})-\tfrac{1}{2}a(\lambda_{\bar{\mathrm{v}}}\lambda_{\bar{\mathrm{v}}'}\overline{\Lambda}_2)\dot{T}_{\mathrm{vv'ec\bar{v}'\bar{v}}}(\widetilde{\Lambda}_1\overline{\Lambda}_2\overline{\Lambda})-a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}'}\Lambda_1)\\
&\times\ddot{T}_{\mathrm{vev'c\bar{v}\bar{v}'}}(\widetilde{\Lambda}_1\overline{\Lambda}_2\overline{\Lambda})\}]+(-1)^{\lambda_{\mathrm{e}}-\lambda_{\bar{\mathrm{v}}}}[(-1)^{\lambda_{\mathrm{c}}+\lambda_{\bar{\mathrm{v}}'}}Y'_{\mathrm{vv'e\bar{v}}}(\tau_1\Lambda_1\Lambda\Lambda_3\Lambda_2)T_{\mathrm{evv'\bar{v}c\bar{v}'}}(\Lambda_2\tau_1)\\
&+a(\lambda_{\mathrm{v}}\lambda_{\mathrm{v}'}\Lambda_2)Y_{\mathrm{v\bar{v}'\bar{v}c}}(\Lambda_1\Lambda_2\Lambda\Lambda_3\tau_1)T_{\mathrm{vev'c\bar{v}\bar{v}'}}(\Lambda_1\tau_1)]+\tfrac{1}{2}\textstyle\sum_u[(-1)^{\lambda_{\mathrm{e}}-\lambda_{\bar{\mathrm{v}}}}a(\lambda_{\mathrm{v}}\lambda_{\mathrm{v}'}\Lambda_1)\\
&\times I_{\mathrm{vev'\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\widetilde{T'}_{\mathrm{v'evc\bar{v}\bar{v}'}}(u\tau_2)+a(\lambda_{\mathrm{v}'}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)I_{\mathrm{vv'e\bar{v}c\bar{v}'}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\\
&\times\widetilde{T'}_{\mathrm{evv'\bar{v}'c\bar{v}}}(u\tau_2)],
\end{aligned}
\tag{C.13a}
$$

$$
\begin{aligned}
&\Omega^{(2)-}_{\mathrm{vv'e\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{c}}-\varepsilon_{\mathrm{vv'e}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}[\widetilde{T}_{\bar{\mathrm{v}}\mathrm{c}\bar{\mathrm{v}}'\mathrm{ev}'}(\Lambda_2\Lambda_1\Lambda)-\tfrac{1}{2}a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)\widetilde{T}_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{cev}'}(\Lambda_2\Lambda_1\Lambda)\\
&+\textstyle\sum_{\overline{\Lambda}_1\overline{\Lambda}_2\overline{\Lambda}}a(\lambda_{\mathrm{v}}\lambda_{\mathrm{v}'}\overline{\Lambda}_2)\{a(\lambda_{\bar{\mathrm{v}}}\lambda_{\bar{\mathrm{v}}'}\overline{\Lambda}_1)T_{\mathrm{c\bar{v}\bar{v}'ev'}}(\widetilde{\overline{\Lambda}}_2\overline{\Lambda}_1\overline{\Lambda})I'_{\mathrm{vv'e\bar{v}c\bar{v}'}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_1\Lambda_2\overline{\Lambda}\Lambda)\\
&-\tfrac{1}{4}a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}\overline{\Lambda}_1)\widetilde{T}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{cev}'}(\overline{\Lambda}_2\overline{\Lambda}_1\overline{\Lambda})I'_{\mathrm{vv'e\bar{v}\bar{v}'c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_1\Lambda_2\overline{\Lambda}\Lambda)\}].
\end{aligned}
\tag{C.13b}
$$

$$
\begin{aligned}
&\Omega^{(2)+}_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{c}}-\varepsilon_{\mathrm{ee'v}})\\
&=\delta_{\Lambda\Lambda_3}\delta_{MM_3}[\tfrac{1}{2}\{\widetilde{\ddot{T}}_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)+\widetilde{\dot{T}}_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)\}-a(\lambda_{\mathrm{e'}}\lambda_{\mathrm{v}}\Lambda_1)\\
&\times\{\widetilde{\ddot{T}}_{\mathrm{eve'\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)+\widetilde{\dot{T}}_{\mathrm{eve'\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda)\}+a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)\textstyle\sum_{\overline{\Lambda}_2\overline{\Lambda}}J_{\mathrm{e\bar{v}'\bar{v}c}}(\overline{\Lambda}\,\overline{\Lambda}_2\Lambda\Lambda_2\Lambda_1)\\
&\times\{\tfrac{1}{2}\ddot{T}_{\mathrm{ee'vc\bar{v}\bar{v}'}}(\widetilde{\Lambda}_1\overline{\Lambda}_2\overline{\Lambda})-a(\lambda_{\mathrm{e'}}\lambda_{\mathrm{v}}\Lambda_1)(\tfrac{1}{2}\widetilde{\ddot{T}}_{\mathrm{eve'c\bar{v}\bar{v}'}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda})+\widetilde{\dot{T}}_{\mathrm{eve'c\bar{v}\bar{v}'}}(\Lambda_1\overline{\Lambda}_2\overline{\Lambda}))\}]\\
&+\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_3\tau_1}\delta_{\Lambda 0}\widetilde{T}_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\Lambda_1\tau_1)+a(\lambda_{\mathrm{e}}\lambda_{\bar{\mathrm{v}}}\Lambda_1)(-1)^{\Lambda_2}Y_{\mathrm{e\bar{v}'\bar{v}c}}(\Lambda_1\Lambda_2\Lambda\Lambda_3\tau_1)\\
&\times T_{\mathrm{ee'vc\bar{v}\bar{v}'}}(\Lambda_1\tau_1)+\textstyle\sum_u[\tfrac{1}{2}a(\lambda_{\mathrm{e'}}\lambda_{\bar{\mathrm{v}}}u)\{I_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_1\Lambda u)T_{\mathrm{vee'c\bar{v}\bar{v}'}}(u\tau_1)\\
&+I_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)T'_{\mathrm{yee'c\bar{v}\bar{v}'}}(u\tau_2)\}+a(\lambda_{\mathrm{e'}}\lambda_{\mathrm{v}}\Lambda_1)\{a(\lambda_{\mathrm{v}}\lambda_{\bar{\mathrm{v}}}u)a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)\\
&\times I_{\mathrm{eve'\bar{v}c\bar{v}'}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\widetilde{T'}_{\mathrm{e'ev\bar{v}'\bar{v}c}}(u\tau_2)+\tfrac{1}{2}(-1)^{\lambda_{\mathrm{e}}-\lambda_{\bar{\mathrm{v}}}}I_{\mathrm{eve'\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\\
&\times\widetilde{T'}_{\mathrm{e'vec\bar{v}\bar{v}'}}(u\tau_2)\}],
\end{aligned}
\tag{C.14a}
$$

$$
\begin{aligned}
&\Omega^{(2)-}_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{c}}-\varepsilon_{\mathrm{ee'v}})\\
&=-\delta_{\Lambda\Lambda_3}\delta_{MM_3}[a(\lambda_{\mathrm{e'}}\lambda_{\mathrm{v}}\Lambda_1)\{\widetilde{T}_{\bar{\mathrm{v}}\mathrm{c}\bar{\mathrm{v}}'\mathrm{ee'v}}(\Lambda_2\Lambda_1\Lambda)-\tfrac{1}{2}a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)\widetilde{T}_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{cee'v}}(\Lambda_2\Lambda_1\Lambda)\}\\
&+\textstyle\sum_{\overline{\Lambda}_1\overline{\Lambda}_2\overline{\Lambda}}a(\lambda_{\mathrm{e}}\lambda_{\mathrm{e'}}\overline{\Lambda}_1)a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}\overline{\Lambda}_2)\{(-1)^{\Lambda_2}I'_{\mathrm{ee'v\bar{v}c\bar{v}'}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_1\Lambda_2\overline{\Lambda}\Lambda)T_{\mathrm{c\bar{v}\bar{v}'vee'}}(\widetilde{\overline{\Lambda}}_2\overline{\Lambda}_1\overline{\Lambda})\\
&+\tfrac{1}{4}I'_{\mathrm{ee'v\bar{v}\bar{v}'c}}(\overline{\Lambda}_1\overline{\Lambda}_2\Lambda_1\Lambda_2\overline{\Lambda}\Lambda)\widetilde{T}_{\bar{\mathrm{v}}'\bar{\mathrm{v}}\mathrm{cvee'}}(\overline{\Lambda}_2\overline{\Lambda}_1\overline{\Lambda})\}].
\end{aligned}
\tag{C.14b}
$$

C.4 Four-body part

$$
\begin{aligned}
&\Omega^{(2)}_{\mathrm{vv'v''v'''\bar{v}\bar{v}'cc'}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{cc'}}-\varepsilon_{\mathrm{vv'v''v'''}})\\
&=\tfrac{1}{2}(-1)^{\Lambda_3}a(\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}\Lambda_1)F_{\mathrm{c'c\bar{v}\bar{v}'}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)Q_{\mathrm{vv'v''v'''\bar{v}cc'\bar{v}'}}(\widetilde{\Lambda}_1\Lambda_3).
\end{aligned}
\tag{C.15}
$$

$$
\begin{aligned}
&\Omega^{(2)}_{\mathrm{evv'v''\bar{v}\bar{v}'cc'}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{cc'}}-\varepsilon_{\mathrm{evv'v''}})\\
&=\tfrac{1}{4}\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_3\Lambda_4}\delta_{\Lambda 0}Q_{\mathrm{evv'v''\bar{v}\bar{v}'cc'}}(\widetilde{\Lambda}_1\Lambda_3)+(-1)^{\Lambda_3}a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}}\Lambda_1)F_{\mathrm{c'c\bar{v}\bar{v}'}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)\\
&\times Q_{\mathrm{vev'v''c\bar{v}c'\bar{v}'}}(\widetilde{\Lambda}_1\Lambda_3)+\tfrac{1}{2}(-1)^{\Lambda_3}a(\lambda_{\mathrm{e}}\lambda_{\mathrm{v}}\Lambda_4)F_{\mathrm{evv'v''}}(\Lambda_4\Lambda_3\Lambda_2\Lambda_1\Lambda)Q_{\mathrm{vv'ev''cc'\bar{v}\bar{v}'}}(\Lambda_4\Lambda_2)\\
&+\tfrac{1}{2}\textstyle\sum_{ud}G_{\mathrm{evv'v''\bar{v}\bar{v}'cc'}}(ud\Lambda_1\Lambda_3\Lambda_2\Lambda_4\Lambda)\widetilde{Q}_{\mathrm{vv'ev''\bar{v}cc'\bar{v}'}}(ud).
\end{aligned}
\tag{C.16}
$$

$$
\begin{aligned}
&\Omega^{(2)}_{\mathrm{ee'vv'\bar{v}\bar{v}'cc'}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)(\varepsilon_{\bar{\mathrm{v}}\bar{\mathrm{v}}'\mathrm{cc'}}-\varepsilon_{\mathrm{ee'vv'}})\\
&=\tfrac{1}{4}\delta_{\Lambda_1\Lambda_2}\delta_{\Lambda_3\Lambda_4}\delta_{\Lambda 0}\{Q_{\mathrm{ee'vv'\bar{v}\bar{v}'cc'}}(\widetilde{\Lambda}_1\Lambda_3)+Q_{\mathrm{vv'ee'cc'\bar{v}\bar{v}'}}(\widetilde{\Lambda}_3\Lambda_1)\}-\tfrac{1}{2}(-1)^{\Lambda_3}\\
&\times\{F_{\mathrm{c'c\bar{v}\bar{v}'}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)Q_{\mathrm{ee'vv'c\bar{v}c'\bar{v}'}}(\widetilde{\Lambda}_1\Lambda_3)+(-1)^{\Lambda_1+\Lambda_4}F_{\mathrm{e'evv'}}(\Lambda_4\Lambda_3\Lambda_2\Lambda_1\Lambda)\\
&\times Q_{\mathrm{eve'v'cc'\bar{v}\bar{v}'}}(\widetilde{\Lambda}_4\Lambda_2)+a(\lambda_{\bar{\mathrm{v}}}\lambda_{\bar{\mathrm{v}}'}\Lambda_2)a(\lambda_{\mathrm{c}}\lambda_{\mathrm{c}'}\Lambda_4)F_{\mathrm{cc'\bar{v}'\bar{v}}}(\Lambda_1\Lambda_2\Lambda_3\Lambda_4\Lambda)\\
&\times Q_{\mathrm{vv'ee'c\bar{v}c'\bar{v}'}}(\widetilde{\Lambda}_3\Lambda_1)+a(\lambda_{\mathrm{v}}\lambda_{\mathrm{v}'}\Lambda_3)a(\lambda_{\mathrm{e}}\lambda_{\mathrm{e'}}\Lambda_4)F_{\mathrm{ee'v'v}}(\Lambda_4\Lambda_3\Lambda_2\Lambda_1\Lambda)\\
&\times Q_{\mathrm{eve'v'\bar{v}\bar{v}'cc'}}(\widetilde{\Lambda}_2\Lambda_4)\}+a(\lambda_{\mathrm{e}}\lambda_{\mathrm{e'}}\Lambda_1)\textstyle\sum_{ud}a(\lambda_{\mathrm{c'}}\lambda_{\bar{\mathrm{v}}'}d)\widetilde{Q}_{\mathrm{eve'v'\bar{v}c\bar{v}'c'}}(ud)\\
&\times G_{\mathrm{e'evv'\bar{v}\bar{v}'cc'}}(ud\Lambda_1\Lambda_3\Lambda_2\Lambda_4\Lambda).
\end{aligned}
\tag{C.17}
$$

Tab. 40: Phase factors $\mathcal{Z}_{\alpha'\beta'\bar{\mu}'\bar{\nu}'}$

$\lambda_{\alpha'}$	$\lambda_{\beta'}$	$\lambda_{\bar{\mu}'}$	$\lambda_{\bar{\nu}'}$	$\mathcal{Z}_{\alpha'\beta'\bar{\mu}'\bar{\nu}'}(\Lambda_1\Lambda_2\Lambda)$
λ_α	λ_β	$\lambda_{\bar{\mu}}$	$\lambda_{\bar{\nu}}$	1
λ_α	λ_β	$\lambda_{\bar{\nu}}$	$\lambda_{\bar{\mu}}$	$a(\lambda_{\bar{\mu}}\lambda_{\bar{\nu}}\Lambda_2)$
λ_β	λ_α	$\lambda_{\bar{\mu}}$	$\lambda_{\bar{\nu}}$	$a(\lambda_\alpha\lambda_\beta\Lambda_1)$
λ_β	λ_α	$\lambda_{\bar{\nu}}$	$\lambda_{\bar{\mu}}$	$a(\lambda_\alpha\lambda_\beta\Lambda_1)\ a(\lambda_{\bar{\mu}}\lambda_{\bar{\nu}}\Lambda_2)$
$\lambda_{\bar{\mu}}$	$\lambda_{\bar{\nu}}$	λ_α	λ_β	$a(\lambda_\alpha\lambda_\beta\Lambda_2)\ a(\lambda_{\bar{\mu}}\lambda_{\bar{\nu}}\Lambda_1)$
$\lambda_{\bar{\mu}}$	$\lambda_{\bar{\nu}}$	λ_β	λ_α	$a(\lambda_{\bar{\mu}}\lambda_{\bar{\nu}}\Lambda_1)$
$\lambda_{\bar{\nu}}$	$\lambda_{\bar{\mu}}$	λ_α	λ_β	$a(\lambda_\alpha\lambda_\beta\Lambda_2)$
$\lambda_{\bar{\nu}}$	$\lambda_{\bar{\mu}}$	λ_β	λ_α	1

The coefficients J, Y, Y', I, I', F, G are defined by the following formulas

$$J_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\overline{\Lambda}_1\overline{\Lambda}_2\Lambda) \stackrel{\text{def}}{=} (-1)^{\Lambda_2+\overline{\Lambda}_2}[\Lambda_1][\Lambda_2,\overline{\Lambda}_2]^{1/2}\begin{Bmatrix}\lambda_\alpha & \lambda_{\bar{\nu}} & \Lambda_1\\ \lambda_{\bar{\mu}} & \lambda_\beta & \Lambda_2\\ \overline{\Lambda}_1 & \overline{\Lambda}_2 & \Lambda\end{Bmatrix}, \tag{C.18a}$$

$$Y_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\overline{\Lambda}_1\overline{\Lambda}_2\Lambda) \stackrel{\text{def}}{=} (-1)^{\Lambda_1+\Lambda_2+\overline{\Lambda}_1+\overline{\Lambda}_2}[\overline{\Lambda}_1,\Lambda_2,\Lambda]^{1/2}$$
$$\times\langle\Lambda M\overline{\Lambda}_1\overline{M}_1|\overline{\Lambda}_2\overline{M}_2\rangle\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \overline{\Lambda}_1\\ \lambda_{\bar{\nu}} & \lambda_{\bar{\mu}} & \lambda_\beta\end{Bmatrix}\begin{Bmatrix}\overline{\Lambda}_1 & \overline{\Lambda}_2 & \Lambda\\ \lambda_\alpha & \lambda_{\bar{\nu}} & \lambda_{\bar{\mu}}\end{Bmatrix}, \tag{C.18b}$$

$$Y'_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\overline{\Lambda}_1\overline{\Lambda}_2\Lambda) \stackrel{\text{def}}{=} (-1)^{\Lambda_1+\Lambda_2}[\Lambda_1,\overline{\Lambda}_1,\Lambda_2]^{1/2}$$
$$\times\langle\Lambda_1 M_1\overline{\Lambda}_1\overline{M}_1|\overline{\Lambda}_2\overline{M}_2\rangle\begin{Bmatrix}\overline{\Lambda}_1 & \Lambda_2 & \Lambda\\ \lambda_\beta & \lambda_\alpha & \lambda_{\bar{\mu}}\end{Bmatrix}\begin{Bmatrix}\overline{\Lambda}_1 & \overline{\Lambda}_2 & \Lambda_1\\ \lambda_{\bar{\nu}} & \lambda_{\bar{\mu}} & \lambda_\alpha\end{Bmatrix}, \tag{C.18c}$$

$$I_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(\Lambda_1\Lambda_2\overline{\Lambda}_1\overline{\Lambda}_2\Lambda\overline{\Lambda}) \stackrel{\text{def}}{=} (-1)^{\Lambda+\overline{\Lambda}_1}[\Lambda_1,\Lambda_2,\overline{\Lambda}_2,\Lambda,\overline{\Lambda}]^{1/2}$$
$$\times\langle\overline{\Lambda}_2\overline{M}_2\Lambda M|\overline{\Lambda}_1\overline{M}_1\rangle\begin{Bmatrix}\lambda_\alpha & \lambda_\beta & \overline{\Lambda}\\ \lambda_{\bar{\nu}} & \lambda_{\bar{\mu}} & \overline{\Lambda}_1\end{Bmatrix}\begin{Bmatrix}\lambda_\beta & \lambda_\zeta & \Lambda_1\\ \lambda_{\bar{\nu}} & \lambda_{\bar{\eta}} & \Lambda_2\\ \overline{\Lambda}_1 & \overline{\Lambda}_2 & \Lambda\end{Bmatrix}, \tag{C.18d}$$

$$I'_{\alpha\beta\zeta\bar{\mu}\bar{\nu}\bar{\eta}}(\Lambda_1\Lambda_2\overline{\Lambda}_1\overline{\Lambda}_2\Lambda\overline{\Lambda}) \stackrel{\text{def}}{=} (-1)^{\lambda_\alpha+\lambda_\zeta+\lambda_{\bar{\mu}}+\lambda_{\bar{\eta}}+\Lambda_1+\overline{\Lambda}_1+\Lambda_2+\Lambda+\overline{\Lambda}}$$
$$\times[\Lambda][\Lambda_1,\Lambda_2,\overline{\Lambda}_1,\overline{\Lambda}_2]^{1/2}\begin{bmatrix}\overline{\Lambda} & \lambda_\beta & \lambda_{\bar{\eta}} & \Lambda\\ \lambda_{\bar{\mu}} & \overline{\Lambda}_2 & \Lambda_1 & \lambda_\zeta\\ \lambda_\alpha & \Lambda_2 & \overline{\Lambda}_1 & \lambda_{\bar{\nu}}\end{bmatrix}, \tag{C.18e}$$

$$F_{\alpha\beta\zeta\rho}(\Lambda_1\Lambda_2\overline{\Lambda}_1\overline{\Lambda}_2\Lambda) \stackrel{\text{def}}{=} (-1)^{\overline{\Lambda}_2}[\Lambda_2,\overline{\Lambda}_2]^{1/2}\begin{Bmatrix}\Lambda_1 & \Lambda_2 & \Lambda\\ \lambda_\rho & \lambda_\beta & \lambda_\zeta\end{Bmatrix}\begin{Bmatrix}\overline{\Lambda}_1 & \overline{\Lambda}_2 & \Lambda\\ \lambda_\beta & \lambda_\rho & \lambda_\alpha\end{Bmatrix}, \tag{C.18f}$$

$$G_{\alpha\beta\zeta\rho\bar{\mu}\bar{\nu}\bar{\eta}\bar{\sigma}}(\Lambda_1\Lambda_2\overline{\Lambda}_1\overline{\Lambda}_2\overline{\overline{\Lambda}}_1\overline{\overline{\Lambda}}_2\Lambda) \stackrel{\text{def}}{=} (-1)^{\Lambda}a(\lambda_\alpha\lambda_\beta\overline{\Lambda}_1)a(\lambda_{\bar{\nu}}\lambda_{\bar{\sigma}}\Lambda_2)$$
$$\times[\Lambda_1,\Lambda_2,\overline{\Lambda}_1,\overline{\Lambda}_2,\overline{\overline{\Lambda}}_1,\overline{\overline{\Lambda}}_2]^{1/2}\begin{Bmatrix}\lambda_\beta & & \lambda_{\bar{\mu}} & \overline{\Lambda}_1 & & \overline{\overline{\Lambda}}_1 & \lambda_\alpha & & \lambda_{\bar{\nu}}\\ & \Lambda_1 & & & \Lambda & & & \Lambda_2 & \\ \lambda_\zeta & & \lambda_{\bar{\eta}} & \overline{\Lambda}_2 & & \overline{\overline{\Lambda}}_2 & \lambda_\rho & & \lambda_{\bar{\sigma}}\end{Bmatrix}, \tag{C.18g}$$

where the last quantity—the $15j$–symbol of the third kind—is defined according to Ref. [10, Sec. 4-20, p. 207, Eq. (20.3)]. In Eqs. (C.3)-(C.8), the expressions for $\mathcal{Z}_{\alpha'\beta'\bar{\mu}'\bar{\nu}'}(\Lambda_1\Lambda_2\Lambda)$, where $\{\alpha',\beta',\bar{\mu}',\bar{\nu}'\}$ denotes somehow permuted orbitals $\{\alpha,\beta,\bar{\mu},\bar{\nu}\}$ of the coefficient $\Omega^{(2)}_{\alpha\beta\bar{\mu}\bar{\nu}}(\Lambda_1\Lambda_2\Lambda)$, are displayed in Tab. 40. Particularly, the abbreviation $\mathcal{Z}_{\alpha'\beta'\bar{\mu}'\bar{\nu}'}(\Lambda_1\Lambda_1 0) \equiv \mathcal{Z}_{\alpha'\beta'\bar{\mu}'\bar{\nu}'}(\Lambda_1)$ is used.

D Symbolic computations with *NCoperators*

The «Non-Commutative operators» package runs under *Mathematica* [99–101], a computational software program. To take all advantage of *NCoperators*, especially when manipulating with the antisymmetric tensors, a free ware package *NCAlgebra* developed by Helton, Stankus et. al. [102] must be compiled. The *NCoperators* package has been written for Unix OS, but it is easy to adapt it for Windows OS as well if some of the parameters of compilation are changed.

The *NCoperators* is a composition of a large number of packages with extension `*.m` that can be divided into four main blocks:

1. Second Quantisation Representation (SQR)
2. Angular Momentum Theory (AMT)
3. Rayleigh–Schrödinger Perturbation Theory (RSPT)
4. Unstructured External Programming (UEP)

The packages store *Mathematica* codes that are loaded into a *Mathematica* session by using the function «"NCoperators.m" or Get["NCoperators.m"]. The *NCoperators* is designed so that each block can be brought into action separately. This is easily done with Get["PackageName.m"]. All these functions (Get[]) are located in a single package NCoperators.m.

D.1 SQR and AMT blocks

The SQR and AMT blocks are closely related and therefore they will be considered together. The present blocks contain a huge number of functions, each of them being useful for a special case of interest. In the present overview, only a few of them will be discussed.

In theoretical atomic physics, a typical task is to find the angular coefficients that relate two distinct momenta coupling schemes. Consider, for example, the momenta recoupling coefficient $\left(j_1 j_2 (j_{12}) j_3 j \middle| j_2 j_3 (j_{23}) j_1 j\right)$. The expression is known, and it is

$$(-1)^{2j+j_2+j_3-j_{23}} [j_{12}, j_{23}]^{1/2} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix}.$$

Making use of *NCoperators*, the algorithm to obtain the latter formula is displayed in Fig. 1.

```
In[25]:= CGcoeff[{j1, m1}, {j2, m2}, {j12, m12}] CGcoeff[{j12, m12}, {j3, m3}, {j, m}]

Out[25]= ⎡ j1  j2  j12 ⎤ ⎡ j12  j3  j ⎤
         ⎣ m1  m2  m12 ⎦ ⎣ m12  m3  m ⎦

In[26]:= Recoupling[%, {j2, m2}, {j3, m3}]

Out[26]= SymbolSum[(-1)^(j+j1+j2+j3) ⎡ j1  j2,j3  j ⎤ ⎡ j2  j3  j2,j3 ⎤ ⎧ j1  j2  j12   ⎫ √(1+2 j12) √(1+2 j2,j3), {j2,j3, m2,m3}]
                                     ⎣ m1  m2,m3  m ⎦ ⎣ m2  m3  m2,m3 ⎦ ⎩ j3  j   j2,j3 ⎭

In[27]:= % /. {j2,j3 → j23, m2,m3 → m23}

Out[27]= SymbolSum[(-1)^(j+j1+j2+j3) ⎡ j1  j23  j ⎤ ⎡ j2  j3  j23 ⎤ ⎧ j1  j2  j12 ⎫ √(1+2 j12) √(1+2 j23), {j23, m23}]
                                     ⎣ m1  m23  m ⎦ ⎣ m2  m3  m23 ⎦ ⎩ j3  j   j23 ⎭

In[28]:= Make[%, {{j23, m23}, {j1, m1}}, {{j2, m2}, {j3, m3}}]

Out[28]= SymbolSum[(-1)^(2 j+j2+j3-j23) ⎡ j2  j3  j23 ⎤ ⎡ j23  j1  j ⎤ ⎧ j1  j2  j12 ⎫ √(1+2 j12) √(1+2 j23), {j23, m23}]
                                        ⎣ m2  m3  m23 ⎦ ⎣ m23  m1  m ⎦ ⎩ j3  j   j23 ⎭

In[29]:= % //. SumSimplify

Out[29]= √(1+2 j12) SymbolSum[(-1)^(2 j+j2+j3-j23) ⎡ j2  j3  j23 ⎤ ⎡ j23  j1  j ⎤ ⎧ j1  j2  j12 ⎫ √(1+2 j23), {j23, m23}]
                                                   ⎣ m2  m3  m23 ⎦ ⎣ m23  m1  m ⎦ ⎩ j3  j   j23 ⎭

In[30]:= % /. style

Out[30]= √(1+2 j12) SymbolSum[(-1)^(2 j+j2+j3-j23) ⎡ j2  j3  j23 ⎤ ⎡ j23  j1  j ⎤ ⎧ j1  j2  j12 ⎫ √(1+2 j23), {j23, m23}]
                                                   ⎣ m2  m3  m23 ⎦ ⎣ m23  m1  m ⎦ ⎩ j3  j   j23 ⎭

In[31]:= % // MakeSymbolSum

Out[31]= ∑j23 ∑m23 (-1)^(2 j+j2+j3-j23) ⎡ j2  j3  j23 ⎤ ⎡ j23  j1  j ⎤ ⎧ j1  j2  j12 ⎫ √(1+2 j23) √(1+2 j12)
                                        ⎣ m2  m3  m23 ⎦ ⎣ m23  m1  m ⎦ ⎩ j3  j   j23 ⎭
```

Fig. 1: A computation of recoupling coefficient $\left(j_1 j_2 (j_{12}) j_3 j \middle| j_2 j_3 (j_{23}) j_1 j\right)$ with *NCoperators*

Out[25] contains two Clebsch–Gordan coefficients labelled by CGcoeff[] – the standard *Mathematica* function ClebschGordan[] is insufficient for symbolic manipulations. The function Recoupling[] initiates the momenta recoupling followed by Refs. [10–12]. SymbolSum[] plays a role of a standard *Mathematica* function Sum[] adapted to symbolic computations. The function Make[] initiates the momenta recoupling within a given Clebsch–Gordan coefficient. The simplification of considered sum is performed by SumSimplify. Out[31] is printed in a standard Unix output form specified by the font family «cmmi10». Obtained formula is easy to convert to a LaTeX language by making use of *Mathematica* function

`Export["DirectoryName/FileName.tex",%31]`. A brief description of all functions is lited by using `Definition[function]` or simply `?function`. The example is presented in Fig. 2.

```
In[45]:= ?TAntiCommutator1

TAntiCommutator1[o_,
{Subscript[λ1_, Subscript[α_,
    i_]], Subscript[m1_, Subscript[α_, i_]]},
{Subscript[λ2_, Subscript[β_, j_]], Subscript[m2_,
    Subscript[β_, j_]]} uses the relationship:

TCreatOp[λ1, m1, i, α] ** TCreatOp[λ2, m2, j, β] =
    -TCreatOp[λ2, m2, j, β] ** TCreatOp[λ1, m1, i, α].
```

Fig. 2: The usage of `Definition[]` in *NCoperators*

In Fig. 2, the function `TAntiCommutator1[]` along with `TAntiCommutator2[]`, `TAntiCommutator3[]` and `TAntiCommutator4[]` initiates the (four) anticommutation rules for irreducible tensor operators $a^{\lambda_{\alpha_i}}_{m_{\alpha_i}}$, $\tilde{a}^{\lambda_{\alpha_i}}_{m_{\alpha_i}}$ (RSPT block). To compare with, the anticommutation properties of the Fock space operators a_{α_i}, $a^{\dagger}_{\alpha_i}$ are realised through the *NCoperators* functions `AntiCommutator1[]`, `AntiCommutator2[]`, `AntiCommutator3[]` and `AntiCommutator4[]`. The examples are listed in Fig. 3. Particularly, `In[61]` computes the one-body terms $\{\widehat{O}_2(\alpha\beta)\widehat{O}_1(\mu\nu)\}_2$ which are found in the Wick's series for $\widehat{h}^{(3)}_{mn;\xi}$ with the indices $m=2$, $n=1$, $\xi=2$ (refer to Eqs. (2.42), (4.3)); `NonCommutOpMulti[n,α,β]` is nothing else but $\widehat{O}_n(\alpha\beta)$. In addition, the function `NonCommutOpMulti[n,α,β,m,μ,ν]` corresponds to $\widehat{O}_n(\alpha\beta)\widehat{O}_m(\mu\nu)$.

```
In[58]:= NonCommutOpMulti[4, α, β]
Out[58]= a_α1 ** a_α2 ** a†_β2 ** a†_β1

In[59]:= AntiCommutator2[%, {α, 2}, {β, 2}] //. Trule
Out[59]= -a_α1 ** a†_β2 ** a_α2 ** a†_β1 + a_α1 ** a†_β1 δ_α,β

In[60]:= % /. style
Out[60]= -a_α1 a†_β2 a_α2 a†_β1 + a_α1 a†_β1 δ_α,β

In[61]:= TwoContractions221[4, α, β, 2, μ, ν]
Out[61]= 2 a_α2 ** a†_β2 δ_α1,ν1 δ_β1,μ1 - 2 a_α1 ** a†_β2 δ_α2,ν1 δ_β1,μ1 - 2 a_α2 ** a†_β1 δ_α1,ν1 δ_β2,μ1 + 2 a_α1 ** a†_β1 δ_α2,ν1 δ_β2,μ1

In[62]:= % /. style
Out[62]= 2 a_α2 a†_β2 δ_α1,ν1 δ_β1,μ1 - 2 a_α1 a†_β2 δ_α2,ν1 δ_β1,μ1 - 2 a_α2 a†_β1 δ_α1,ν1 δ_β2,μ1 + 2 a_α1 a†_β1 δ_α2,ν1 δ_β2,μ1
```

Fig. 3: Manipulations with the antisymmetric Fock space operators in *NCoperators*

```
In[78]:= MatrixEl[α, v, β]
Out[78]= ⟨α | v | β⟩

In[79]:= WignerEckart[%, {j, m}, {k, q}]
Out[79]= ( j_β  k  j_α ) [j_α ‖v^(k)‖ j_β]
         ( m_β  q  m_α )
```

Fig. 4: Wigner–Eckart theorem in *NCoperators*

There are many more functions in *NCoperators*. Many tasks in atomic physics are related to the Wigner–Eckart theorem. This theorem is also found in the present package. The example of usage is demonstrated in Fig. 4, where the projection-independent quantity $\left[j_\alpha \| v^{(k)} \| j_\beta\right]$ denotes a usual reduced matrix element of the irreducible tensor operator $v^{(k)}$. Note, throughout the present text, the notation v^k is preferred.

D.2 RSPT block

The present block involves functions suitable for the symbolic manipulations observed in the stationary Rayleigh–Schrödinger perturbation theory. In principal, the RSPT block applies the previously summarised blocks with some specific functions particular with the MBPT. Without going into too much details concerned with the structure of programmed codes, consider an example related to the third-order MBPT (Sec. 4). Select the one-body term $\widehat{h}^{(3)}_{11;1}\colon\ \mathcal{P}\longrightarrow\mathcal{P}$. By Eq. (4.3),

$$\widehat{h}^{(3)}_{11;1} =: \{\widehat{P}\widehat{V}_1\widehat{\Omega}^{(2)}_1\widehat{P}\}_1 : \,.$$

The operators $\widehat{V}_1\colon\ \mathfrak{F}\longrightarrow\mathfrak{F}$, $\widehat{\Omega}^{(2)}_1\colon\ \mathcal{P}\longrightarrow\mathcal{H}$ given by Eqs. (2.40), (2.69a) are deduced to be equal to

$$\widehat{V}_1 = \sum_{\alpha\beta} a_\alpha a^\dagger_{\bar\beta} v_{\alpha\bar\beta}, \quad \widehat{\Omega}^{(2)}_1 = \sum_{\mathrm{ev}} a_{\mathrm{e}} a^\dagger_{\bar{\mathrm{v}}} \omega^{(2)}_{\mathrm{e}\bar{\mathrm{v}}} + \sum_{\mathrm{vc}} a_{\mathrm{v}} a^\dagger_{\bar{\mathrm{c}}} \omega^{(2)}_{\mathrm{v}\bar{\mathrm{c}}} + \sum_{\mathrm{ec}} a_{\mathrm{e}} a^\dagger_{\bar{\mathrm{c}}} \omega^{(2)}_{\mathrm{e}\bar{\mathrm{c}}},$$

where the single-particle matrix element $v_{\alpha\bar\beta}$ is defined in Eq. (4.5). Recall that only the types of single-electron orbitals are written below the sums, but not their values.

```
In[2]:= A111 // Clear
        A111 :=
          Block[{x1, x2, x3, x4, x4a, x5, x6, x7, x8},
           x1 = 1 / 1 * (
                  P ** NormalOrder[OneContraction[2, μ, ν, 2, vc1, ca1]] ** P * MatrixEl[μ1, ν1, ν1] * MatrixEl[vc1₁, ν2, ca1₁] /
                     (ε_ca1₁ - ε_vc1₁) +
                   P ** NormalOrder[OneContraction[2, μ, ν, 2, ec1, ca1]] ** P * MatrixEl[μ1, ν1, ν1] *
                    MatrixEl[ec1₁, ν2, ca1₁] /
                     (ε_ca1₁ - ε_ec1₁) +
                   P ** NormalOrder[OneContraction[2, μ, ν, 2, ec1, va1]] ** P * MatrixEl[μ1, ν1, ν1] *
                    MatrixEl[ec1₁, ν2, va1₁] /
                     (ε_va1₁ - ε_ec1₁)) /. {KronDelta[μ1, va1_] :> 0, KronDelta[μ2, va1_] :> 0} //. Trule // Expand;
           x2 = Table[SymbolSum[ x1[[i]], {μ1, ν1}] //. SumSimplify, {i, 1, Length[x1]}] // Total;
           x3 = (x2 /. {μ → vc2, ν → va2}) + (x2 /. {μ → ec2, ν → ea2}) + (x2 /. {μ → cc2, ν → ca2});
           x4 = x3 /. {a___ * SymbolSum[z__, var_List] :> a * z};
           x5 = x4 //. Elimination;
           x6 = (x5 // NormalOrdering) /. P → 1;
           x7 = x6 /. {v1 → ν1, v2 → ν2^eff} /. style /. style /. style /. style /. style /. style
          ];

In[4]:= A111

Out[4]= - a_m1 a†_p2 ⟨a2|v1|p2⟩⟨m1|v2^eff|a2⟩ / (ε_a2 - ε_m1) + a_p1 a†_m2 ⟨r1|v2^eff|m2⟩⟨p1|v1|r1⟩ / (ε_m2 - ε_r1)
```

Fig. 5: The generation of $\widehat{h}^{(3)}_{11;1}$ terms with *NCoperators*

In Fig. 5, the generation of $\widehat{h}^{(3)}_{11;1}$ terms is demonstrated. Many of the functions in Fig. 5 are easy to detect by their names: `NormalOrder[]` denotes ::; `OneContraction[]` denotes the one-pair contractions ($\xi = 1$) between $\widehat{V}_1$ and $\widehat{\Omega}^{(2)}_1$; `KronDelta[]` is obviously the Kronecker delta function. Other supplementary functions are to be used for various technical simplifications. In `Out[4]`, $\langle a|v_2^{eff}|b\rangle \equiv \omega^{(2)}_{ab}(\varepsilon_b - \varepsilon_a)$ (recall the irrep τ_2) and $\langle a|v_1|b\rangle \equiv v_{ab}$ (recall the irrep τ_1).

In *NCoperators*, the three types—core (c), valence (v), excited (e)—of single-electron orbitals are designated by

$$\begin{array}{llll} a_{\mathrm{c}}: & \mathrm{cc1}, \mathrm{cc2}, \text{etc.}; & a^\dagger_{\bar{\mathrm{c}}}: & \mathrm{ca1}, \mathrm{ca2}, \text{etc.} \\ a_{\mathrm{v}}: & \mathrm{vc1}, \mathrm{vc2}, \text{etc.}; & a^\dagger_{\bar{\mathrm{v}}}: & \mathrm{va1}, \mathrm{va2}, \text{etc.} \\ a_{\mathrm{e}}: & \mathrm{ec1}, \mathrm{ec2}, \text{etc.}; & a^\dagger_{\bar{\mathrm{e}}}: & \mathrm{ea1}, \mathrm{ea2}, \text{etc.} \end{array}$$

In a standard output (such as `Out[4]`), the notations of orbitals are simplified to

$$\begin{array}{llll} \mathrm{c}: & a_1,b_1,c_1,d_1,e_1,f_1 & \bar{\mathrm{c}}: & a_2,b_2,c_2,d_2,e_2,f_2 \\ \mathrm{v}: & m_1,n_1,p_1,q_1,k_1,l_1 & \bar{\mathrm{v}}: & m_2,n_2,p_2,q_2,k_2,l_2 \\ \mathrm{e}: & r_1,s_1,t_1,u_1,w_1,x_1 & \bar{\mathrm{e}}: & r_2,s_2,t_2,u_2,w_2,x_2 \end{array}$$

Therefore, in accordance with Fig. 5, the generated terms $\widehat{h}^{(3)}_{11;1}$ are

$$\widehat{h}^{(3)}_{11;1} = \sum_{\mathrm{ev}} a_{\mathrm{v}} a^{\dagger}_{\bar{\mathrm{v}}} v_{\mathrm{ve}} \omega^{(2)}_{\mathrm{e}\bar{\mathrm{v}}} - \sum_{\mathrm{cv}} a_{\mathrm{v}} a^{\dagger}_{\bar{\mathrm{v}}} v_{\mathrm{c}\bar{\mathrm{v}}} \omega^{(2)}_{\mathrm{vc}}. \tag{D.1}$$

The next step is to restrict the model space $\mathcal{P}$ to its irreducible subspaces $\mathcal{P}^{\Lambda}$, that is, to expand $\widehat{h}^{(3)}_{11;1}$ into the sum of irreducible tensor operators $W^{\Lambda}(\lambda_{\mathrm{v}}\widetilde{\lambda}_{\bar{\mathrm{v}}})$. Refer to Eqs. (4.4), (4.17a). Consider the operators $\widehat{h}^{(3)+}_{11;1}$ associated to $\omega^{(2)+}_{\alpha\bar{\beta}}$. In this case, it is easily done by using the expression for SU(2)–invariant in the first row of Tab. 12: simply replace $f(\tau_2\lambda_\mu\lambda_{\bar{\beta}})/(\varepsilon_{\bar{\beta}}-\varepsilon_\mu)$ with $\Omega^{(2)+}_{\mu\bar{\beta}}(\Lambda)$ (recall Remark 4.1.1). But the present invariant has been obtained also making use of *NCoperators*. Thus, for the sake of clarity, the full procedure of angular reduction will be demonstrated. This is, however, easy to perform.

In Eq. (D.1), the first term contains the product of type $\sum_\mu v_{\alpha\mu}\omega^{(2)+}_{\mu\bar{\beta}}$, while the second one – the product of type $\sum_\mu v_{\mu\bar{\beta}}\omega^{(2)+}_{\alpha\mu}$. These products determine the single-particle effective matrix elements. Then

$$\begin{aligned} \sum_{\mathrm{e}} v_{\mathrm{ve}}\omega^{(2)+}_{\mathrm{e}\bar{\mathrm{v}}} &= \sum_{\lambda_{\mathrm{e}}m_{\mathrm{e}}} (-1)^{\lambda_{\mathrm{e}}+m_{\mathrm{e}}} f(\tau_1\lambda_{\mathrm{v}}\lambda_{\mathrm{e}}) \langle \lambda_{\mathrm{v}} m_{\mathrm{v}} \lambda_{\mathrm{e}} - m_{\mathrm{e}} | \tau_1 m_1 \rangle \\ &\quad \times (-1)^{\lambda_{\bar{\mathrm{v}}}+m_{\bar{\mathrm{v}}}} \sum_{\Lambda} \Omega^{(2)+}_{\mathrm{e}\bar{\mathrm{v}}}(\Lambda) \langle \lambda_{\mathrm{e}} m_{\mathrm{e}} \lambda_{\bar{\mathrm{v}}} - m_{\bar{\mathrm{v}}} | \Lambda M \rangle, \\ \sum_{\mathrm{c}} v_{\mathrm{c}\bar{\mathrm{v}}}\omega^{(2)+}_{\mathrm{vc}} &= \sum_{\lambda_{\mathrm{c}}m_{\mathrm{c}}} (-1)^{\lambda_{\bar{\mathrm{v}}}+m_{\bar{\mathrm{v}}}} f(\tau_1\lambda_{\mathrm{c}}\lambda_{\bar{\mathrm{v}}}) \langle \lambda_{\mathrm{c}} m_{\mathrm{c}} \lambda_{\bar{\mathrm{v}}} - m_{\bar{\mathrm{v}}} | \tau_1 m_1 \rangle \\ &\quad \times (-1)^{\lambda_{\mathrm{c}}+m_{\mathrm{c}}} \sum_{\Lambda} \Omega^{(2)+}_{\mathrm{vc}}(\Lambda) \langle \lambda_{\mathrm{v}} m_{\mathrm{v}} \lambda_{\mathrm{c}} - m_{\mathrm{c}} | \Lambda M \rangle. \end{aligned}$$

Finally, recalling that $a_{\mathrm{v}}a^{\dagger}_{\bar{\mathrm{v}}} = (-1)^{\lambda_{\bar{\mathrm{v}}}+m_{\bar{\mathrm{v}}}} \sum_\Lambda W^{\Lambda}_{M}(\lambda_{\mathrm{v}}\widetilde{\lambda}_{\bar{\mathrm{v}}}) \langle \lambda_{\mathrm{v}} m_{\mathrm{v}} \lambda_{\bar{\mathrm{v}}} - m_{\bar{\mathrm{v}}} | \Lambda M \rangle$, the expression in the first row of Tab. 15 (the case $m = n = \xi = 1$) is obtained by using the result in Fig. 1.

A much more complicated task is to find $\Omega^{(2)+}_{\alpha\bar{\beta}}(\Lambda)$. To generate the single-particle effective matrix elements $\omega^{(2)}_{\alpha\bar{\beta}}$, make use of the generalised Bloch equation in Eq. (4.2). It follows that $\omega^{(2)}_{\alpha\bar{\beta}}$ is the sum of $\omega^{(2)}_{ij;i+j-1}(\alpha\bar{\beta})$ $\forall i,j = 1,2$, where the coefficients $\omega^{(2)}_{ij;i+j-1}(\alpha\bar{\beta})$ are obtained from the terms

$$:\{\widehat{R}\widehat{V}_i\widehat{\Omega}^{(1)}_j\widehat{P} - \widehat{R}\widehat{\Omega}^{(1)}_j\widehat{P}\widehat{V}_i\widehat{P}\}_{i+j-1}: .$$

The operator $\widehat{R}$—also known as the resolvent [34]—is defined here by the action on some functional $\mathscr{F}(x^{\dagger}_{f_1}, x^{\dagger}_{f_2}, \ldots, x^{\dagger}_{f_a}, x_{i_1}, x_{i_2}, \ldots, x_{i_a})$ on $\mathcal{H}$ so that

$$\widehat{R}\mathscr{F}(x^{\dagger}_{f_1}, x^{\dagger}_{f_2}, \ldots, x^{\dagger}_{f_a}, x_{\bar{f}_1}, x_{\bar{f}_2}, \ldots, x_{\bar{f}_a}) = \left[\mathscr{D}_a(f\bar{f})\right]^{-1}\widehat{Q}\mathscr{F}(x^{\dagger}_{f_1}, x^{\dagger}_{f_2}, \ldots, x^{\dagger}_{f_a}, x_{\bar{f}_1}, x_{\bar{f}_2}, \ldots, x_{\bar{f}_a}).$$

The energy denominator $\mathscr{D}_a(f\bar{f})$ is found from Eq. (2.65); the vectors $x_{\bar{f}_k}$ $(x^{\dagger}_{f_k})$ $\forall k = 1,2,\ldots,a$ of the single-particle Hilbert space are identified to be the single-particle eigenstates $|\bar{f}_k\rangle$ $(\langle f_k|)$.

The example how to generate the $\omega^{(2)}_{11;1}$ terms is demonstrated in Figs. 6-7: in Fig. 6, the terms $\{\widehat{R}\widehat{V}_1\widehat{\Omega}^{(1)}_1\widehat{P}\}_1$ are generated, while in Fig. 7, the terms $\{\widehat{R}\widehat{\Omega}^{(1)}_1\widehat{P}\widehat{V}_1\widehat{P}\}_1$ are derived. As a result, $\omega^{(2)}_{11;1}$ contains 9 expansion terms

$$\omega^{(2)}_{11;1}(\alpha\bar{\beta})(\varepsilon_{\bar{\beta}}-\varepsilon_\alpha) = \sum_{\mu(\alpha\beta)} v_{\alpha\mu}\omega^{(1)}_{\mu\bar{\beta}} - \sum_{\nu(\alpha\beta)} v_{\nu\bar{\beta}}\omega^{(1)}_{\alpha\nu},$$

```
In[16]:= RV1Ω1PconnectedOnePair // Clear
RV1Ω1PconnectedOnePair = Block[{w1, w2, w3, w4, w5, w6, w7, w8, w9, w10, w11, w12, w13, w14, w15},
   w1[α_, β_] := NormalOrder[OneContraction[2, α, β, 2, ec2, ca2]] * MatrixEl[ec2_1, v_2, ca2_1] / Δ[2, ec2, ca2] +
     NormalOrder[OneContraction[2, α, β, 2, ec2, va2]] * MatrixEl[ec2_1, v_2, va2_1] / Δ[2, ec2, va2] +
     NormalOrder[OneContraction[2, α, β, 2, vc2, ca2]] * MatrixEl[vc2_1, v_2, ca2_1] / Δ[2, vc2, ca2];
   w2[α_, β_] := w1[α, β] // Expand;
   w3[α_, β_] := w2[α, β] * MatrixEl[α_1, v_1, β_1] // Expand;
   w4[β_] := (w3[α, β] /. {α -> ec1}) + (w3[α, β] /. {α → vc1}) + (w3[α, β] /. {α → cc1});
   w5 = (w4[β] /. {β → ea1}) + (w4[β] /. {β → va1}) + (w4[β] /. {β → ca1});
   w6 = w5 // Expand;
   w7 = w6 /. {
       KronDelta[Subscript[ec1, k_], Subscript[ea2, l_]] :→ 0,
       KronDelta[Subscript[vc1, k_], Subscript[va2, l_]] :→ 0,
       KronDelta[Subscript[ca1, k_], Subscript[cc2, l_]] :→ 0};
   w8 = Table[Q ** w7[[f]] ** P, {f, 1, Length[w7]}] // Total;
   w9 = (w8 //. MBPTrules) //. PQrules;
   w10 = w9 // NormalOrdering;
   w11 = w10 //. Elimination;
   w12 = (w11 / δε) // Expand;
   w13 = w12 //. denominator11;
   w14 = Table[RenameState[w13[[i]], {cc1_1, ca1_1, ec1_1, ea1_1, vc1_1, va1_1, cc2_1, ca2_1, ec2_1, ea2_1, vc2_1, va2_1}],
       {i, 1, Length[w13]}] // Total;
   w15 = w14 //. WaveOpSimplify //. WaveOpSimplify2

  ];

In[18]:= (SymbolSum[RV1Ω1PconnectedOnePair, {ca2_1, ea1_1, va1_1}] //. SumExpand //. SumSimplify) /. {
            SymbolSum[z____, var_List] :→ z} /. P → 1 /. Q → 1 /. style /. style /. style /. style /. style
```

$$\text{Out[18]}= -\frac{a_{p_1} a^\dagger_{a_2} \langle a_1|v_1|a_2\rangle\langle p_1|v_2|a_1\rangle}{(\varepsilon_{a_1}-\varepsilon_{p_1})(\varepsilon_{a_2}-\varepsilon_{p_1})} + \frac{a_{m_1} a^\dagger_{c_2} \langle m_1|v_1|p_1\rangle\langle p_1|v_2|c_2\rangle}{(\varepsilon_{c_2}-\varepsilon_{m_1})(\varepsilon_{c_2}-\varepsilon_{p_1})} + \frac{a_{r_1} a^\dagger_{c_2} \langle r_1|v_1|p_1\rangle\langle p_1|v_2|c_2\rangle}{(\varepsilon_{c_2}-\varepsilon_{p_1})(\varepsilon_{c_2}-\varepsilon_{r_1})} - \frac{a_{t_1} a^\dagger_{a_2} \langle a_1|v_1|a_2\rangle\langle t_1|v_2|a_1\rangle}{(\varepsilon_{a_1}-\varepsilon_{t_1})(\varepsilon_{a_2}-\varepsilon_{t_1})} +$$
$$\frac{a_{m_1} a^\dagger_{c_2} \langle t_1|v_2|c_2\rangle\langle m_1|v_1|t_1\rangle}{(\varepsilon_{c_2}-\varepsilon_{m_1})(\varepsilon_{c_2}-\varepsilon_{t_1})} + \frac{a_{r_1} a^\dagger_{c_2} \langle r_1|v_1|t_1\rangle\langle t_1|v_2|c_2\rangle}{(\varepsilon_{c_2}-\varepsilon_{r_1})(\varepsilon_{c_2}-\varepsilon_{t_1})} - \frac{a_{t_1} a^\dagger_{m_2} \langle a_1|v_1|m_2\rangle\langle t_1|v_2|a_1\rangle}{(\varepsilon_{a_1}-\varepsilon_{t_1})(\varepsilon_{m_2}-\varepsilon_{t_1})} + \frac{a_{r_1} a^\dagger_{p_2} \langle r_1|v_1|t_1\rangle\langle t_1|v_2|p_2\rangle}{(\varepsilon_{p_2}-\varepsilon_{r_1})(\varepsilon_{p_2}-\varepsilon_{t_1})}$$

Fig. 6: The generation of $\omega^{(2)}_{11;1}$ terms: part 1

```
In[19]:= RΩ1PV1POnePair // Clear
RΩ1PV1POnePair = Block[{w1, w2, w3, w4, w5, w6, w7, w8, w9, w10, w11, w12, w13, w14, w15},
   w1[μ_, ν_] := NormalOrder[OneContraction[2, ec2, ca2, 2, μ, ν]] * MatrixEl[ec2_1, v_2, ca2_1] / Δ[2, ec2, ca2] +
     NormalOrder[OneContraction[2, ec2, va2, 2, μ, ν]] * MatrixEl[ec2_1, v_2, va2_1] / Δ[2, ec2, va2] +
     NormalOrder[OneContraction[2, vc2, ca2, 2, μ, ν]] * MatrixEl[vc2_1, v_2, ca2_1] / Δ[2, vc2, ca2];
   w2[μ_, ν_] := w1[μ, ν] // Expand;
   w3[μ_, ν_] := w2[μ, ν] * MatrixEl[μ_1, v_1, ν_1] // Expand;
   w4[ν_] := w3[μ, ν] /. {μ → vc1};
   w5 = w4[v] /. {v → va1};
   w6 = w5 // Expand;
   w7 = w6 /. {
       KronDelta[Subscript[ec1, k_], Subscript[ea2, l_]] :→ 0,
       KronDelta[Subscript[vc1, k_], Subscript[va2, l_]] :→ 0,
       KronDelta[Subscript[ca1, k_], Subscript[cc2, l_]] :→ 0,
       KronDelta[Subscript[ec2, k_], Subscript[ea1, l_]] :→ 0,
       KronDelta[Subscript[vc2, k_], Subscript[va1, l_]] :→ 0,
       KronDelta[Subscript[ca2, k_], Subscript[cc1, l_]] :→ 0
      };
   w8 = (Q ** (w7 // NormalOrdering) ** P) //. MBPTrulesExpand;
   w9 = (w8 //. MBPTrules) //. PQrules;
   w10 = w9 //. Elimination;
   w11 = (w10 / δε) // Expand;
   w12 = w11 //. denominator11;
   w13 = RenameState[w12, {cc1_1, ca1_1, ec1_1, ea1_1, vc1_1, va1_1, cc2_1, ca2_1, ec2_1, ea2_1, vc2_1, va2_1}];
   w14 = w13 //. WaveOpSimplify //. WaveOpSimplify2

  ];

In[21]:= (SymbolSum[RΩ1PV1POnePair, {va2_1}] //. SumSimplify) /. P → 1 /. Q → 1 /. style /. style /. style /. style
```

$$\text{Out[21]}= \frac{a_{t_1} a^\dagger_{m_2} \langle t_1|v_2|m_1\rangle\langle m_1|v_1|m_2\rangle}{(\varepsilon_{m_1}-\varepsilon_{t_1})(\varepsilon_{m_2}-\varepsilon_{t_1})}$$

Fig. 7: The generation of $\omega^{(2)}_{11;1}$ terms: part 2

where $\mu(\mathrm{vc}) = \mu(\mathrm{ec}) = \mathrm{v},\mathrm{e}$; $\mu(\mathrm{ev}) = \mathrm{e}$; $\nu(\mathrm{vc}) = \nu(\mathrm{ec}) = \mathrm{c}$; $\nu(\mathrm{ev}) = \mathrm{v},\mathrm{c}$. Analogous computations must be performed for the rest of coefficients $\omega^{(2)}_{12;2}$, $\omega^{(2)}_{21;2}$, $\omega^{(2)}_{22;3}$, and thus

$$\omega^{(2)}_{\alpha\bar\beta} = \omega^{(2)}_{11;1}(\alpha\bar\beta) + \omega^{(2)}_{12;2}(\alpha\bar\beta) + \omega^{(2)}_{21;2}(\alpha\bar\beta) + \omega^{(2)}_{22;3}(\alpha\bar\beta),$$

where

$$\begin{aligned}
\omega^{(2)}_{12;2}(\alpha\bar\beta)(\varepsilon_{\bar\beta} - \varepsilon_\alpha) &= \sum_{\mathrm{c}} \sum_{\mu=\mathrm{v},\mathrm{e}} v_{\mathrm{c}\mu} \widetilde{\omega}^{(1)}_{\mu\alpha\mathrm{c}\bar\beta}, \\
\omega^{(2)}_{21;2}(\alpha\bar\beta)(\varepsilon_{\bar\beta} - \varepsilon_\alpha) &= \sum_{\mathrm{c}} \sum_{\mu=\mathrm{v},\mathrm{e}} \widetilde{v}_{\mathrm{c}\alpha\mu\bar\beta} \omega^{(1)}_{\mu\mathrm{c}}, \\
\omega^{(2)}_{22;3}(\alpha\bar\beta)(\varepsilon_{\bar\beta} - \varepsilon_\alpha) &= \sum_{\mathrm{c},\mathrm{v},\mathrm{e}} \widetilde{v}_{\mathrm{c}\alpha\mathrm{ve}} \widetilde{\omega}^{(1)}_{\mathrm{evc}\bar\beta}.
\end{aligned}$$

The expressions are identified in Tab. 12, where the corresponding $\mathrm{SU}(2)$–invariants are selected (recall the distinct notations for distinct intermediate irreps defined by Eqs. (4.11)-(4.16)). Then split the solution for $\omega^{(2)}_{\alpha\bar\beta}$ into the sum of $\omega^{(2)+}_{\alpha\bar\beta}$ and $\omega^{(2)-}_{\alpha\bar\beta}$. Make use of Eq. (4.17a). Finally, the solutions for $\Omega^{(2)\pm}_{\alpha\bar\beta}$ are displayed in Eqs. (C.1)-(C.2) in Appendix C.

The algorithm of generation and angular reduction of $\widehat{h}^{(3)}_{11;1}$ terms is suited to the rest of operators $\widehat{h}^{(3)}_{mn;\xi}$. It is by no means obvious that the procedure to find out the effective matrix elements associated to $\widehat{\Omega}^{(2)}_n$ with $n \geq 2$ is much more complicated, though the idea holds true for all of them:

$$\begin{aligned}
n=2: &\quad \omega^{(2)}_{\alpha\beta\bar\mu\bar\nu} = \textstyle\sum_{i,j=1}^{2} \omega^{(2)}_{ij;i+j-2}(\alpha\beta\bar\mu\bar\nu), && \widehat{\Omega}^{(2)}_2 = :\{\widehat{R}\widehat{V}_i\widehat{\Omega}^{(1)}_j\widehat{P} - \widehat{R}\widehat{\Omega}^{(1)}_j\widehat{P}\widehat{V}_i\widehat{P}\}_{i+j-2}:, \\
n=3: &\quad \omega^{(2)}_{\alpha\beta\zeta\bar\mu\bar\nu\bar\eta} = \textstyle\sum_{i,j=1}^{2} \omega^{(2)}_{ij;i+j-3}(\alpha\beta\zeta\bar\mu\bar\nu\bar\eta), && \widehat{\Omega}^{(2)}_3 = :\{\widehat{R}\widehat{V}_i\widehat{\Omega}^{(1)}_j\widehat{P} - \widehat{R}\widehat{\Omega}^{(1)}_j\widehat{P}\widehat{V}_i\widehat{P}\}_{i+j-3}:, \\
n=4: &\quad \omega^{(2)}_{\alpha\beta\zeta\rho\bar\mu\bar\nu\bar\eta\bar\sigma} = \omega^{(2)}_{22;0}(\alpha\beta\zeta\rho\bar\mu\bar\nu\bar\eta\bar\sigma), && \widehat{\Omega}^{(2)}_4 = :\widehat{R}\widehat{V}_2\widehat{\Omega}^{(1)}_2\widehat{P}: - :\widehat{R}\widehat{\Omega}^{(1)}_2\widehat{P}\widehat{V}_2\widehat{P}:,
\end{aligned}$$

assuming that for $\xi = 2,3$, the condition $i + j - \xi \geq 0$ is valid.

D.3 UEP block

The present block is the most technical one, as it is closely related to the operating system used. The UEP block has been designed for the Unix systems and it can be skipped for those who are keen on other systems. Nevertheless, the block actualises many useful features, though it is still permanently augmented. The main idea is to convert obtained symbolic preparation into the C code for a more rapid calculation of the quantities under consideration.

External programming is a way of communication between *Mathematica* interface and some other (external) programs (such as C). Differently from the structured programming actualised by using *MathLink*, the unstructured programming does not require any other external «tunnels» except for the user's own terminal.

```
f[n_, x_, y_, z_] := (-1)^n * SixJ[{x, y, z}, {x, y, z}],

f[1, 15., 14., 15.] // Timing // Chop // N
{0.024001, -0.00146234}

Cfunction[f, float, {n, x, y, z}, {1, 15., 14., 15.},
  {int, float, float, float}] // Timing
{0.016001, -0.0014623}

f[1, 35., 34., 35.] // Timing // Chop // N
{0.036002, 0.000417085}

Cfunction[f, float, {n, x, y, z}, {1, 35., 34., 35.},
  {int, float, float, float}] // Timing
{0.004, 0.0004171}
```

Fig. 8: Example of an application of the UEP block

To make the UEP block operate, the *Mathematica* header file *mdefs.h* must be located in the directory, where all system header files are situated. In most Unix systems, the directory is *usr/include/*. The header is supplemented with the C-based functions that are necessary for the atomic calculations: `ClebschGordanC[]`, `SixJSymbolC[]`, `NineJSymbolC[]`, etc. The *MathLink* libraries *libML32i3.a*, *libML32i.so* are substituted in */usr/lib* or */usr/local/lib*.

The example of the usage of C-based functions within *Mathematica* interface is demonstrated in Fig. 8, where the function

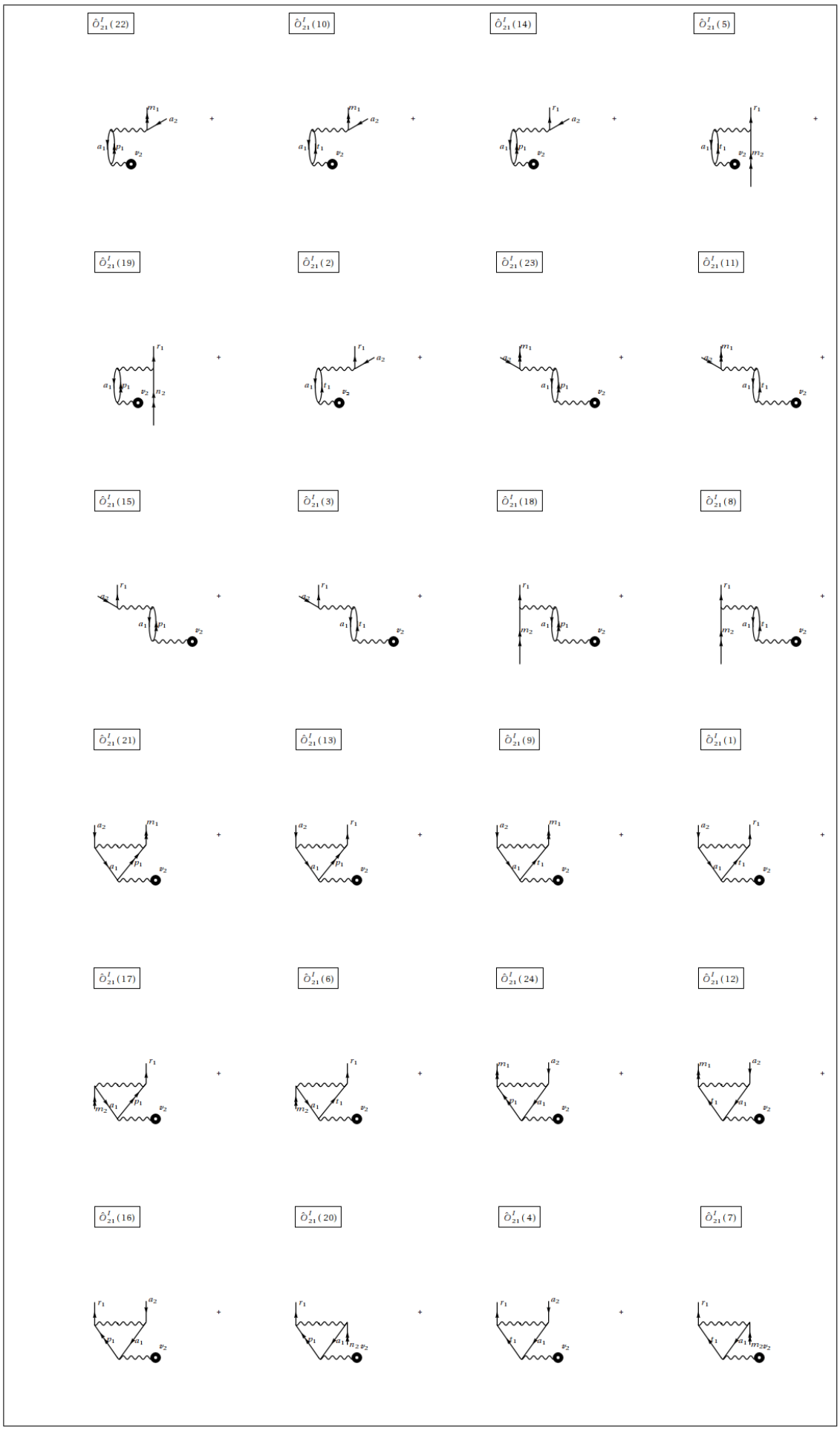

Fig. 9: The diagrammatic visualisation of :$\{\widehat{R}\widehat{V}_2\widehat{\Omega}_1^{(1)}\widehat{P}\}_2$: terms

`Timing[]` clearly demonstrates the main benefit of such type of programming that stipulates, therefore, the further on improvements in the same direction.

Perspectives In addition to the briefly studied possibilities of the application of *NCoperators*, one more option can be found in the present package. It is a diagrammatic visualisation of expansion terms. The example is demonstrated in Fig. 9. A newbie equipment of *NCoperators* is actualised by using the *Mathematica* functions `Graphics[]`, `Show[]`. Likewise in the case of UEP block, the present feature is not fully operational at this time.

The diagrammatic visualisation has the only one advantage to compare with the algebraic formulation of atomic MBPT. It is an easy to behold visualisation of complex algebraic expressions. It is not a mere mnemonic device, though. A number of rules to handle the diagrams designed for atomic and nuclear spectroscopy are formulated. However, as demonstrated in Sec. 4, such visualisation is inefficient due to a huge number of expansion terms. Consequently, there are two alternatives: whether to write programs that are capable to visualise expansion terms diagrammatically and afterwards to convert them into a usual algebraic form or to take aim at the algebraic approach such as developed in Sec. 4. The *NCoperators* package has been designed to be of versatile disposition as much as it is possible. Therefore, the direction that must be chosen strongly depends on the future demands.

References

[1] N. Bohr, Philosophical Magazine **26**, 1 (1913)

[2] Maria G. Mayer, Phys. Rev. A **74**, no. 3, 235 (1948)

[3] Maria G. Mayer, Phys. Rev. A **75**, no. 13, 1969 (1949)

[4] O. Haxel, J. Hans D. Jensen, Hans E. Suess, Phys. Rev. A **75**, no. 11, 1766 (1949)

[5] E. U. Condon, G. H. Shortley, The Theory of Atomic Spectra, Cambridge, Cambridge Univ. Press (1935)

[6] E. P. Wigner, " On the matrices which reduce the Kronecker products of representations of simply reducible groups", in Quantum Theory of Angular Momentum edited by L. C. Biedenharn and J. D. Louck, New York, Academic (1965)

[7] G. Racah, Phys. Rev. **61**, 186 (1942)

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

[9] G. Racah, Phys. Rev. **63**, 367 (1943)

[10] A. Jucys, Y. Levinson and V. Vanagas, Mathematical Apparatus of the Theory of Angular Momentum, Vilnius, 3rd ed. (Russ. Original, Gospolitnauchizdat, 1960)

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

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

[13] D. J. Newman and J. Wallis, J. Phys. A: Math. Gen. **9**, no. 12, 2021 (1976)

[14] G. Gaigalas, Z. Rudzikas and Ch. F. Fischer, J. Phys. B: At. Mol. Opt. Phys. **30**, 3747 (1997)

[15] G. Gaigalas, S. Fritzsche, I. P. Grant, Comput. Phys. Comm. **139**, no. 3, 263 (2001)

[16] G. Gaigalas and S. Fritzsche, Comput. Phys. Comm. **148**, no. 3, 349 (2002)

[17] S. Fritzsche, Comput. Phys. Comm. **180**, no. 10, 2021 (2009)

[18] Ch. F. Fischer, J. Phys. B: At. Mol. Phys. **3**, no. 6, 779 (1970)

[19] M. R. Godefroid, Ch. F. Fischer and P. Jönsson, Phys. Scr. **1996**, T65, 70 (1996)

[20] Ch. F. Fischer, A. Ynnerman, G. Gaigalas, Phys. Rev. A **51**, no. 6, 4611 (1995)

[21] K. A. Brueckner, Phys. Rev. **97**, no. 5, 1344 (1955)

[22] K. A. Brueckner, Phys. Rev. **100**, no. 1, 36 (1955)

[23] J. Goldstone, J. Proc. R. Soc. Lond. A **239**, 267 (1957)

[24] H. P. Kelly, Phys. Rev. **131**, 684 (1963)

[25] H. P. Kelly, Phys. Rev. **134**, A1450 (1964)

[26] H. P. Kelly, Phys. Rev. **144**, 39 (1966)

[27] D. Mukherjee, R. K. Moitra and A. Mukhopadhyay, Mol. Phys. **30**, 1861 (1975)

[28] I. Lindgren, Int. J. Quant. Chem. **S12**, 33 (1978)

[29] J. Morrison and S. Salomonson, Phys. Scr. **21**, 343 (1980)

[30] V. Kvasnička, Chem. Phys. Lett. **79**, no. 1, 89 (1981)

[31] W. Kutzelnigg, Chem. Phys. Lett. **83**, 156 (1981)

[32] I. Lindgren, Phys. Rev. A **31**, no. 3, 1273 (1985)

[33] D. Mukherjee, Chem. Phys. Lett. **125**, no. 3, 207 (1986)

[34] I. Lindgren, J. Morrison, Atomic Many-Body Theory, Springer Series in Chemical Physics, Vol. 13 (1982)

[35] S. A. Blundell, W. R. Johnson and J. Sapirstein, Phys. Rev. A **43**, no. 7, 3407 (1991)

[36] M. S. Safronova, W. R. Johnson and U. I. Safronova, Phys. Rev. A **53**, no. 53, 4036 (1996)

[37] H. C. Ho and W. R. Johnson et. al., Phys. Rev. A **74**, 022510, 1 (2006)

[38] A. Derevianko, J. Phys. B: At. Mol. Opt. Phys. **43**, 074001, 1 (2010)

[39] I. Lindgren and D. Mukherjee, Phys. Rep. **151**, no. 2, 93 (1987)

[40] G. C. Wick, Phys. Rev. **80**, no. 2, 268 (1950)

[41] S. A. Blundell, W. R. Johnson and J. Sapirstein, Phys. Rev. A **42**, no. 7, 3751 (1990)

[42] S. G. Porsev, A. Derevianko, Phys. Rev. A **73**, 012501 (2006)

[43] V. Dzuba, Comput. Phys. Comm. **180**, no. 3, 392 (2009)

[44] http://wolfweb.unr.edu/homepage/andrei/tap.html

[45] Z. Csepes and J. Pipek, J. Comput. Phys. **77**, no. 1, 1 (1988)

[46] B. R. Judd, Operator Techniques in Atomic Spectroscopy, McGraw-Hill, New York (1963)

[47] B. R. Judd, Second Quantization and Atomic Spectroscopy, Baltimore, MD: Johns Hopkins (1967)

[48] B. R. Judd and R. C. Leavitt, J. Phys. B: At. Mol. Phys. **15**, 1457 (1982)

[49] R. C. Leavitt, J. Phys. B: At. Mol. Phys. **21**, 2363 (1987)

[50] Z. Rudzikas, J. Kaniauskas, Quasispin and Isospin in the Theory of Atom, Vilnius, Mokslas Publishers (1984) (in Russian)

[51] J. M. Kaniauskas, V. Č. Šimonis and Z. B. Rudzikas, J. Phys. B: At. Mol. Phys. **20**, 3267 (1987)

[52] Z. Rudzikas, Theoretical Atomic Spectroscopy, Cambridge, Cambridge Univ. Press (1997)

[53] G. Gaigalas, J. Kaniauskas et. al., Phys. Scr. **49**, 135 (1994)

[54] G. Merkelis, Phys. Scr. **61**, 662 (2000)

[55] G. Merkelis, Phys. Scr. **63**, 289 (2001)

[56] C. F. Bunge, At. Data Nucl. Data Tables **18**, 293 (1976)

[57] W. J. Marciano, J. L. Rosner, Phys. Rev. Lett. **65**, 2963 (1990)

[58] J. Sapirstein, K. T. Cheng, Phys. Rev. A **67**, 022512 (2003)

[59] P. Ramond, Group Theory: A Physicist's Survey, Cambridge, Cambridge Univ. Press (2010)

[60] J. C. Slater, Phys. Rev. **34**, no. 10, 1293 (1929)

[61] E. P. Wigner, Group Theory and its Applications to the Quantum Mechanics of Atomic Spectra, New York, Academic Press (1959)

[62] N. J. Vilenkin, Special Functions and the Theory of Group Representations, 2nd ed., Moscow, Nauka (1991) (in Russian)

[63] V. V. Vanagas, Algebraic Foundation of the Microscopic Nuclear Theory, Moscow, Nauka (1988) (in Russian)

[64] A. U. Klimyk, Matrix Elements and Clebsch-Gordan Coefficients of Representations of Groups, Kiev, Naukova Dumka (1979) (in Russian)

[65] A. K. Bhatia, A. Temkin, Rev. Mod. Phys. **36**, 1050 (1964)

[66] R. Juršėnas and G. Merkelis, Int. J. Theor. Phys. **49**, no. 9, 2230 (2010)

[67] Z. B. Rudzikas, J. M. Kaniauskas, Int. J. Quant. Chem. **10**, 837 (1976)

[68] P. R. Smith and B. G. Wybourne, J. Math. Phys. **9**, 1040 (1968)

[69] B. G. Wybourne, Spectroscopic Properties of Rare Earths, New York, John Wiley & Sons, Inc. (1965)

[70] W. Kutzelnigg, Int. J. Quant. Chem. **109**, 3858 (2009)

[71] H. Feshbach, Ann. Phys. (N.Y.) **5**, 357 (1958)

[72] R. Juršėnas and G. Merkelis, At. Data Nucl. Data Tables (2010), doi:10.1016/j.adt.2010.08.001

[73] R. Juršėnas and G. Merkelis, to appear in J. Math. Phys. (2010)

[74] A. Derevianko, S. G. Porsev, Phys. Rev. A **71**, 032509 (2005)

[75] A. Derevianko, S. G. Porsev and K. Beloy, Phys. Rev. A **78**, 010503(R) (2008)

[76] V. Vanagas, Algebraic Methods in Nuclear Theory, Vilnius (1971) (in Russian)

[77] R. Juršėnas, G. Merkelis, Cent. Eur. J. Phys. **8**, no. 3, 480 (2010)

[78] R. Juršėnas and G. Merkelis, MPM e-journal **9**, no. 1, 42 (2010)

[79] W. Fulton, J. Harris, Representation Theory: A First Course, New York, Springer-Verlag Inc. (1991)

[80] R. Juršėnas, G. Merkelis, Cent. Eur. J. Phys. (2010), doi:10.2478/s11534-010-0082-0

[81] R. Juršėnas and G. Merkelis, Lithuanian J. Phys. **47**, no. 3, 255 (2007)

[82] M. A. Braun, A. D. Gurchumelia, U. I. Safronova, Relativistic Atom Theory, Moscow, Nauka (1984) (in Russian)

[83] G. Breit, Phys. Rev. **35**, 569 (1930)

[84] A. A. Nikitin, Z. B. Rudzikas, Foundations of the Theory of the Spectra of Atoms and Ions, Moscow, Nauka (1983) (in Russian)

[85] J. M. Kaniauskas, V. V. Špakauskas, Z. B. Rudzikas, Lietuvos Fizikos Rinkinys **19**, no. 1, 21 (1979) (in Russian)

[86] G. V. Merkelis, G. A. Gaigalas, Z. B. Rudzikas, Lietuvos Fizikos Rinkinys **25**, no. 6, 14 (1985) (in Russian)

[87] G. Merkelis, Nucl. Instr. Meth. Phys. Research B **235**, 184 (2005)

[88] R. Pal et. al., Phys. Rev. A **74**, 042515 (2007)

[89] B. R. Judd, Phys. Rev. **141**, 4 (1966)

[90] H. Dothe et. al. J. Phys. B: At. Mol. Phys. **18**, 1061 (1985)

[91] P. H. M. Uylings, J. Phys. B: At. Mol. Phys. **17**, 2375 (1984)

[92] J. Noga and R. J. Barllet, Chem. Phys. Lett. **134**, no. 2, 126 (1987)

[93] L. Meissner, P. Malinowski and J. Gryniakow, J. Phys. B: At. Mol. Phys. **37**, 2387 (2004)

[94] Sh. Matsumoto and J. Novak, DMTCS proc., 403 (2010)

[95] T. Graber and R. Vakil, Compositio Math. **135**, no. 1, 25 (2003)

[96] A. A. Jucys, Lietuvos Fizikos Rinkinys **11**, no. 1, 5 (1971) (in Russian)

[97] A. A. Jucys, Rep. Math. Phys. **5**, 107 (1974)

[98] G. E. Murphy, J. Algebra **69**, 287 (1981)

[99] S. Wolfram, The Mathematica Book, Wolfram Media, Cambridge Univ. Press, 4th ed. (1999)

[100] http://www.wolfram.com/

[101] A. Dargys, A. Acus, Fizika su kompiuteriu, Ciklonas, Vilnius (2003) (in Lithuanian)

[102] http://www.math.ucsd.edu/~ncalg/