Development of algebraic techniques for the atomic open-shell MBPT(3)

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The atomic third-order open-shell many-body perturbation theory is developed. Special attention is paid to the generation and algebraic analysis of terms of the wave operator and the effective Hamiltonian as well. Making use of occupation-number representation and intermediate normalization, the third-order deviations are worked out by employing a computational software program that embodies the generalized Bloch equation. We prove that in the most general case, the terms of effective interaction operator on the proposed complete model space are generated by not more than eight types of the $n$-body ($n \geq 2$) parts of the wave operator. To compose the effective Hamiltonian matrix elements handily, the operators are written in irreducible tensor form. We present the reduction scheme in a versatile disposition form, thus it is suited for the coupled-cluster approach.

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I. INTRODUCTION

From the mathematical point of view, many-body perturbation theory (MBPT) is represented by a number of recurrence equations which permit to construct a total wave function of many-body system up to the fixed amendment. The higher order excitations are involved, the larger number of corrections is found. Due to interactions of the valence electrons, this number drastically increases for open-shell atoms. Over the past decades, it has become generally accepted to build the wave operator which maps states in selected model space onto exact states of complex system Hamiltonian, upon the generalized Bloch equation, introduced by Lindgren et. al. Although, the practical application of this equation is far from being as mere as the theory is. The situation exceptionally changed, when symbolic programming tools appropriated sufficiently high level. Particularly, we exclude a computational software program Mathematica. There exist several symbolic packages, written to evaluate the diagrams or algebraic expressions of MBPT. Nevertheless, the specific features, necessary in computations, are known, as a rule, to the authors only. Therefore we developed the symbolic package NCopertors, and the computational part of the present study relies on this package. The package has been tested by generating the terms of the first-order wave operator and the second-order effective Hamiltonian.

The other two parts of this paper are devoted to the construction of model space and the reduction of generated terms. A good survey to various aspects of the problems that merge the selection of model space can be found in the reports of Lindgren, Kutzelnigg et.al. On the one hand, we follow the traditional MBPT by excluding three types of the one-electron orbitals: core, virtual (or excited) and valence. On the other hand, we propose an algebraic investment that accounts for the operation of valence creation and annihilation operators on the model space in a strict manner (Sec. II). In the result, we formulate a precise statement which determines the amount of Fock space operators by the differing types of one-electron orbitals. That is, it ascertains the terms of the wave operator producing none zero contributions to the effective interaction operator. The theorem enables to simplify algebraic procedure, improving further on analysis (especially reduction) of terms. To apply the suggested formulation of PT, we display all obtained one-body and two-body terms of the third-order effective Hamiltonian in irreducible tensor form (Sec. III). The reduction is performed by using the angular momentum theory. The reduction scheme is presented
in a versatile disposition form, thus it is suited with the coupled-cluster (CC) approach, if some elementary replacements are initiated. Meanwhile, we show how suggested algebraic approach results to a compactness and easily accessible form of terms. The method is based on the construction of effective \( n \)-particle matrix elements, rather than the writing of each algebraic expression side by side its diagrammatic visualization, as, for example, in the classical works of Ho, Lindgren et. al.\(^{2,3,6,17}\) as well as in the recently appeared papers\(^{18–21}\).

II. THE SELECTION OF MODEL SPACE

A. Hilbert space

Suppose given a set \( X \equiv \{ h_k \}_{k=1}^{\infty} \) of orthonormal \( N \)-electron eigenstates \( h_k \) of the central-field Hamiltonian \( H_0 \) with the eigenvalues \( \hat{E}_0 \). The configuration state functions (CSF) \( h_k \) are characterized by the sets \( \{ \Pi_k^X, \Lambda_k, M_k \} \) of numbers: (i) the configuration parity \( \Pi_k^X = \pm 1 \); (ii) the irreducible representations \( \Lambda_k \) of group \( G \), where \( \Lambda_k \equiv L_k S_k \) if \( G = \text{SO}_L(3) \times \text{SU}_S(2) \) and \( \Lambda_k \equiv J_k \) if \( G = \text{SU}(2) \). The indices \( M_k \equiv M_L M_S \) or \( M_k \equiv M_J \) enumerate the basis for \( \Lambda_k \).

By\(^{22}\), we let \( \langle \cdot, \cdot \rangle_\mathcal{H} : X \times X \rightarrow \mathbb{R} \) be a real function, called the scalar product on \( N \)-particle Hilbert space \( \mathcal{H} \), where

\[
\mathcal{H} = \{ h_k : \langle h_k \cdot h_l \rangle_\mathcal{H} = \delta_{kl}, \forall k, l \in \mathbb{Z}^+ \}. \tag{1}
\]

The infinite Hilbert space \( \mathcal{H} \) is assumed to be separable, thus there exist the linear forms \( \Psi(i) \in \mathcal{H} \), the parameter \( \epsilon > 0 \) and the integer \( I_\epsilon \) such that \( \| \Psi(i) - \sum_{k=1}^{M} c_k(i) h_k \|_\mathcal{H} < \epsilon \) for any \( M > I_\epsilon \) and \( c_k(i) \in \mathbb{R}, i = 1, 2, \ldots, D \). If particularly \( M = \infty \), then \( \Psi(i) \) will denote the eigenstates of the \( N \)-electron atomic Hamiltonian \( H = H_0 + V \) with the eigenvalues \( E_i \), where \( V \) represents the perturbation.

Along with the scalar product (or equivalently the norm \( \| , \| = \sqrt{\langle \cdot, \cdot \rangle} \)), we also propose a unit operator on \( \mathcal{H} \).

**Proposition II.1.** The form \( \hat{1} : \mathcal{H} \rightarrow \mathcal{H} \), expressed by

\[
\hat{1} = \sum_{k=1}^{\infty} h_k h_k^+, \tag{2}
\]

is a unit operator on \( N \)-particle Hilbert space \( \mathcal{H} \).
Proof. For the vectors \( h_k \), we immediately gather
\[
\hat{1} h_k = \sum_{l=1}^{\infty} h_l \langle h_l \cdot h_k \rangle_H = h_k.
\]
In \( H \), we may construct various linear forms \( \Psi \equiv \sum_{k=1}^{M} c_k h_k \in H \), \( c_k \in \mathbb{R} \). Thus for the vectors \( \Psi \), we get
\[
\hat{1} \Psi = \sum_{k=1}^{M} c_k \hat{1} h_k = \Psi.
\]
This proves the proposition.

B. Orthogonal subspaces

From the given set \( X \) of orthonormal functions \( h_k \) (Sec. II A), we form a subset \( Y \subset X \) that is formed from the countable functions \( h_k \equiv \phi_k \forall k = 1, 2, \ldots, d < \infty \). We insist the functions \( \phi_k \) to be identified by the sets of numbers \( \{\Pi_Y \Lambda_k M_k\} \). Here the configuration parity \( \Pi_Y \) is identical for all \( \phi_k \), for all \( k = 1, 2, \ldots, d \). The representations \( \Lambda_k \) are obtained by reducing the Kronecker products of irreducible representations \( \lambda \) which in turn label the one-electron orbitals. These orbitals are represented by two types: core (c) and valence (v). We also insist the subset \( Y \) to be complete by means of the allocation of valence orbitals in all possible ways.

Since \( Y = \{\phi_k\}_{k=1}^{d} \) is the subset of vectors of \( H \), it is sufficient to introduce a finite-dimensional subspace \( P \) (dim \( P = d \)) of \( H \) by
\[
P = \{\phi_k : \langle \phi_k \cdot \phi_l \rangle_H = \delta_{kl}, \forall k, l = 1, 2, \ldots, d\}.
\]
Then the orthogonal complement \( P^\perp \equiv Q = H \ominus P \) of \( P \) is defined by
\[
Q = \{\theta_k \equiv h_{d+k} : \langle \theta_k \cdot \theta_l \rangle_H = \delta_{kl}, \forall k, l \in \mathbb{Z}^+\}.
\]
This immediately implies that
\[
\langle \phi_k \cdot \theta_l \rangle_H = 0 \quad \forall k = 1, 2, \ldots, d \quad \forall l \in \mathbb{Z}^+,
\]
thus the orthonormal functions \( \theta_l \) form the complement \( Z = X \setminus Y = \{\theta_l\}_{l=1}^{\infty} \), and they are particularly characterized by the sets of numbers \( \{\Pi^Z_l \Lambda_l M_l\} \). Let us study the properties of \( \theta_l \) that are predetermined by the orthogonality in Eq. (3). First of all, Eq. (3) is true, regardless of whether \( \Pi^Z_l = \Pi_Y \) or not, as \( Z \cap Y = \emptyset \) and \( h_k \in H \) (see Eq. (11)). Secondly, Eq. (5) does not exclude the functions \( \theta_l \) that could contain core and/or valence orbitals of \( \phi_k \) if \( \Pi^Z_l \neq \Pi_Y \). By Eq. (11), on the other hand, we are not confined to form the infinite set \( X \) of functions \( h_k \) in any manner if reserving the formal conditions, presented in Sec. II A.
Considerably, we insist the functions \( \theta_l \) to include the one-electron orbitals that are absent in all \( \phi_k \), irrespectively whether \( \Pi^Z = \Pi^Y \) or not. These orbitals will be called excited (e) or virtual.

C. The model functions

From now on, we assume that the number \( D \) of the selected eigenstates \( \Psi(i) \) of \( H \) equals to \( \dim \mathcal{P} = d \). Then by Prop. I.1,

\[
\hat{\Psi}(i) = \Psi(i) = \sum_{k=1}^{d} \phi_k \langle \phi_k \cdot \Psi(i) \rangle_H + \sum_{l=1}^{\infty} \theta_l \langle \theta_l \cdot \Psi(i) \rangle_H = \Phi(i) + \hat{Q} \Psi(i), \quad \Phi(i) = \hat{P} \Psi(i) = \sum_{k=1}^{d} c_k(i) \phi_k, \tag{6}
\]

where

\[
\hat{P} = \sum_{k=1}^{d} \phi_k \phi_k^\dagger, \quad \hat{Q} = \sum_{l=1}^{\infty} \theta_l \theta_l^\dagger, \quad \hat{P} + \hat{Q} = \hat{1}, \tag{7}
\]

\[
c_k(i) = \langle \phi_k \cdot \Psi(i) \rangle_H = \langle \phi_k \cdot \Phi(i) \rangle_H \in \mathbb{R}. \tag{8}
\]

The functions \( \Phi(i) \) will be called the model functions of \( \mathcal{P} \) (see Ref.6). In Eq. (6), if replacing \( \hat{Q} \) with \( \hat{Q} = (\hat{\Omega} - \hat{1}) \hat{P} \), then we simply get \( \Psi(i) = \hat{\Omega} \Phi(i) \), where \( \hat{\Omega} \) is called the wave operator.

The procedure how to construct the generalized Bloch equation for \( \hat{\Omega} \) is well known and it will not be presented here.

D. The improvement of generation of Hilbert space operators

In this section, we wish to select the rules that allow to generate the terms of the wave operator as well as the effective interaction operator efficiently. As it will be demonstrated later, the rules under consideration significantly improve the computation of terms of higher-order PT.

The wave operator is represented by the infinite series, where the first term is \( \hat{1} \). The rest of terms \( \hat{\Omega}^{(m)} (m \geq 1) \) consist of the sum of \( n \)-body parts \( \hat{\Omega}_n^{(m)} \), where \( n = 1, 2, \ldots \) depends on \( m \). We define \( \hat{\Omega}_n \) (for any \( m \), in general) by
\[ \hat{\Omega}_n = \sum_{\alpha_i, \beta_j} \hat{Q} \hat{O}_n^{(\alpha \beta)} \hat{P} \omega_{\alpha_1 \alpha_2 \ldots \alpha_n \beta_1 \beta_2 \ldots \beta_n}, \]  

\[ \hat{O}_n^{(\alpha \beta)} = a_{\alpha_1} a_{\alpha_2} \ldots a_{\alpha_{n-1}} a_{\alpha_n} a_{\beta_n}^\dagger a_{\beta_{n-1}}^\dagger \ldots a_{\beta_2}^\dagger a_{\beta_1}^\dagger. \]  

In Eq. (9), the summation is performed over all types (e, v, c) of the one-electron orbitals. Hereafter, we do not write in the sum the concrete values of orbitals \((\ldots \alpha_i, \ldots, \beta_j, \ldots)\), only designating their type \((\alpha_i = z_i, \beta_j = z_j, z = e, v, c)\). The quantities \(\omega_{\alpha_1 \ldots \alpha_n \beta_1 \ldots \beta_n}\) denote some structure coefficients, composed of the product of one-particle and/or two-particle matrix elements (energy denominators included). In accordance with Eq. (7), the Fock space operators \(a_\alpha\) (creation) and \(a_{\beta}^\dagger\) (annihilation) are assigned as follows

\[
\begin{align*}
(A) & \quad a_\alpha \hat{P} = 0, & (C) & \quad a_\alpha \hat{P} \neq 0, \\
(B) & \quad a_{\beta}^\dagger \hat{P} = 0, & (D) & \quad a_{\beta}^\dagger \hat{P} \neq 0.
\end{align*}
\]

On the one hand, items (A)-(B) correspond to the definitions, presented in Ref. 6 (Eq. (13.3), p. 288). On the other hand, items (C)-(D) are strictly determined and they realize the arguments (Sec. 13.1.2, p. 288) that it is possible to create as well as annihilate valence electrons in \(\mathcal{P}\). It will be demonstrated later that these items are of special significance. Moreover, items (C)-(D) point to the definition of the complete model space by means of the allocation of valence states in \(\phi_k\) in all possible ways (see Sec. II.B).

The definition of \(\hat{\Omega}_n\) conforms to the elucidation, enunciated in accordance with the generalized Bloch equation (Eq. (11.62), p. 247), as \(\hat{\Omega}_n\) plays a role of operator, connecting \(\hat{Q}\) and \(\hat{P}\) spaces. (In diagrammatic representation \(\hat{\Omega}_n\) includes open diagrams.) Here are the rules which establish the distributions of \(\alpha_i, \bar{\beta}_j\) providing none zero contributions of \(\hat{O}_n^{(\alpha \bar{\beta})}\).

Proposition II.2 (6, p. 292). The operator \(\hat{P} \hat{O}_n^{(\alpha \bar{\beta})} \hat{P} \neq 0\) \(\forall \alpha, \beta = v\).

Proposition II.3. The operator \(\hat{Q} \hat{O}_n^{(\alpha \bar{\beta})} \hat{Q} \neq 0\) \(\forall \alpha, \beta = z\).

Proposition II.4. The operator \(\hat{Q} \hat{O}_n^{(\alpha \bar{\beta})} \hat{P} \neq 0\) \(\forall \alpha = e, v, \forall \beta = v, c\).

By Eq. (10), the self-adjoint operator \(\hat{O}_n^{\dagger (\alpha \bar{\beta})} = \hat{O}_n^{(\bar{\beta} \alpha)}\). Thus, Proposition II.4 may be reformulated in a distinct way.
\textbf{Corollary II.5.} The operator $\hat{P}\hat{O}_n(\alpha\beta)\hat{Q} \neq 0 \forall \alpha = v, c, \forall \beta = e, v$.

The proof of Proposition II.2 is obvious, and it directly follows from Eq. (11).

\textbf{Proof (Proposition II.3.)} It suffices to prove that $\hat{Q}a_\alpha\hat{Q} \neq 0$, since in this case, the expression $\hat{Q}a_\alpha\hat{Q} = (\hat{Q}a_\alpha\hat{Q})^\dagger \neq 0$. By Eq. (11) and the expression $\hat{P} + \hat{Q} = \hat{1}$, we obtain:

1. $\hat{Q}a_\alpha\hat{Q} = \hat{Q}a_\alpha$. But $\hat{Q}a_\alpha = (a_\alpha^\dagger \hat{Q})^\dagger \neq 0$. (2) The operator $\hat{Q}a_\alpha\hat{Q} = a_\alpha\hat{Q} \neq 0$. (3) $\hat{Q}a_\alpha\hat{Q} = [a_\alpha, \hat{P}] \neq 0$, where $[\cdot, \cdot]$ denotes a commutator.

The proof of Proposition II.4 immediately follows from Propositions II.2-II.3, and there is no point to present it here.

Proposition II.3 agrees with the statement of Lindgren (p. 292), if the identity $\alpha = \beta = \nu$ is neglected. The last condition, as a rule, is simply postulated to be false; otherwise, due to zero-valued energy denominators, the infinite terms $\hat{O}_n$ are observed. However, we will study the operators $\hat{Q}\hat{O}_n(\nu^\dagger \nu)\hat{P}$ on the Hilbert space $\mathcal{H}$ in a more detail to show in which cases the rejection of the excluded condition $\alpha = \beta = \nu$ is true, since it has a direct connection to the properties of the model functions $\Phi(i)$ (see Eq. (6)) which form the subspace $\mathcal{P}$ (see Eq. (3)).

Suppose for simplicity that $n = 1$. Also, let us mark (see Sec. II B)

$$\phi_k \equiv h(\lambda_{N_{ki}}^N \lambda_{N_{kj}}^N \ldots \lambda_{N_{ku}}^N \Gamma_k \Pi^Y \Lambda_k M_k), \quad k = 1, 2, \ldots d,$$

where $\lambda_{N_{ki}}^N$ is the $u$th electron shell in $\phi_k$; $\Gamma_k$ denotes additional quantum numbers. Then by Eq. (7), the operator

$$\hat{Q}\hat{O}_1(\nu^\dagger \nu)\hat{P} = \sum_{k=1}^{d} \sum_{l=1}^{\infty} \theta_{l} (\theta_{l} \cdot \phi_k^\dagger)_h \phi_k^\dagger,$$

$$\phi_k^\dagger \equiv a_{v_1}^\dagger a_{v_1}^\dagger \phi_k = (-1)^{j-1} \sum_{i=1}^{N_{ki}^N} N_{ki}^N + \sum_{j=1}^{N_{kj}^N} N_{kj}^N + \delta_{ij} + 1 \delta\lambda_{v_1} \lambda_{ki}$$

$$\times h(n_{k1}^N \lambda_{N_{ki}^N} n_{k2}^N \lambda_{N_{kj}^N} \ldots n_{ki}^N \lambda_{N_{ki}^N} n_{ki}^N \lambda_{N_{ki}^N} n_{ki}^N \lambda_{N_{ki}^N} \ldots$$

$$\ldots n_{kj}^N \lambda_{N_{kj}^N} n_{kj}^N \lambda_{N_{kj}^N} \ldots n_{ku}^N \lambda_{N_{ku}^N} \Pi_k \Lambda_k M_k).$$

The parity of the $N$-electron CSF $\phi_k^\dagger$ equals to $\Pi_k = (-1)^{\delta_{v_1} + \delta_{v_1}^N} \Pi^Y$. It is assumed that $a_{v_1}^\dagger$ and $a_{v_1}$ annihilate and create the $i$th and $j$th valence states of $\phi_k$, respectively. If $\Pi_k = \Pi^Y$, then
then, by the definition of $\mathcal{P}$, obtained functions $h(\ldots)$ on the right hand side of Eq. (13) belong to the set $Y$, and thus

$$
\phi'_k = (-1)^{\sum_{x=1}^{i-1} N_{kx} + \sum_{y=1}^{j-1} N_{ky} + \delta_{ij} + 1} \delta_{\lambda_{\bar{v}1} \lambda_{ki}}, \quad k' = 1, 2, \ldots, d.
$$

Thus for $i = j$, we obtain a particular case $k = k'$, if the shell $\lambda_{ki}^{N_{ki}}$ in $\phi_k$ is labeled by $\lambda_{ki} = \lambda_{\bar{v}}$.

In general, for some $k$, the functions $\phi_k'$ are zeroes. Nevertheless, due to the completeness of the finite set $Y$ (Sec. II B), there will always be at least one function $\phi_k$ with $\lambda_{ki} = \lambda_{\bar{v}}$.

But $\langle \theta_l \cdot \phi_k' \rangle_{\mathcal{H}} = 0, \forall k' = 1, 2, \ldots, d$ (see Eq. (5)). This implies $\hat{Q}\hat{O}_1(v\bar{v})\hat{P} = 0$. The generalization of studied example holds for any $n$.

**Corollary II.6.** The operator $\hat{Q}\hat{O}_n(v\bar{v})\hat{P} = 0$, if $\sum_{i=1}^{n} (l_{vi} + l_{kvi})$ is even for those $k$ values which determine the electron shell $n_{kvi}^{N_{kvi}}$ in $\phi_k \in \mathcal{P}$.

(Obviously, the condition in Corollary II.6 holds for $\hat{P}\hat{O}_n(v\bar{v})\hat{Q}$ too.) In other words, Corollary II.6 represents an additional parity selection rule. The practical treatment of present rule in the study of triple excitations in CC approach can be found in Ref. 18 (Sec. III-E, p. 6).

We can now summarize. The selected $d$-dimensional subspace $\mathcal{P}$ of $N$-electron separable Hilbert space $\mathcal{H}$ is assumed to be constructed of the set $Y$ of same parity configuration state functions $\phi_k$ by allocating the valence electrons in all possible ways (complete model space). Additionally, in order to avoid the divergence of terms of the PT, we select the parity conservation rule in Corollary II.6 to be true. The subspace $\mathcal{P}$ will be called the model space.

Finally, let us define the effective interaction operator by $\mathcal{W}$ (Eq. (15.5), p. 386)

$$
W = \sum_n \sum_{\xi \leq 4} W_{n,\xi} = \sum_n \sum_{\xi \leq 4} \{ \hat{P}(V_1 + V_2)\hat{\Omega}_n\hat{P} \}_\xi,
$$

where $\xi = 1, 2, 3, 4$ denotes the number of contractions between the $i$-body parts ($i = 1, 2$) of perturbation $V$ and the $n$-body parts of $\hat{\Omega}$ (for $n + i - \xi \geq 0$). On behalf of the definition of $\mathcal{P}$, the associated operators $W_{n,\xi}$ are generated by applying the following theorem.

**Theorem II.7.** If the $n$-body part of the wave operator $\hat{\Omega}$ is defined by Eq. (9), then none zero terms of the effective interaction operator $W$ on the model space $\mathcal{P}$ are generated by maximal eight types of the Fock space operators $\hat{O}_n(\alpha\beta)$ for all $n \geq 2$. 

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Possible allocations of $\alpha_i$ and $\bar{\beta}_j$ (see Eq. (11)) orbitals for all $i, j = 1, 2, \ldots, n$ are these:

\[
\begin{align*}
(1) & \quad \begin{cases}
\alpha_1 = e, & \alpha_i = v_i \\
\bar{\beta}_j = v_j \\
i = 2,3,\ldots,n \\
j = 1,2,\ldots,n
\end{cases} \\
(2) & \quad \begin{cases}
\alpha_i = v_i \\
\bar{\beta}_1 = \bar{c}, & \bar{\beta}_j = \bar{v}_j \\
i = 1,2,\ldots,n \\
j = 2,3,\ldots,n
\end{cases} \\
(3) & \quad \begin{cases}
\alpha_1 = e, & \alpha_i = v_i \\
\bar{\beta}_1 = \bar{c}, & \bar{\beta}_j = \bar{v}_j \\
i = 2,3,\ldots,n \\
j = 2,3,\ldots,n
\end{cases}
\]

Because of the anticommutation properties of creation and annihilation operators, the similar allocations of none valence orbitals hold for any selected $i, j$, not only $i, j = 1, 2$.

Theorem III.7 also fits the effective Hamiltonian, given by the formula $H_{\text{eff}}^{(m+1)} = \hat{P}V\hat{\Omega}^{(m)}\hat{P}$. In this case, the structure coefficients $\omega$ in Eq. (9) are replaced with $\omega^{(m)}$, obtained from $\hat{\Omega}^{(m)}$. For $m = 2$, these coefficients will be displayed in the next section, where we examine a special case of the application of proposed formalism.

III. THE THIRD-ORDER EFFECTIVE HAMILTONIAN

In open-shell MBPT, the procedure to determine some fixed number $i = 1, 2, \ldots, d$ of energy levels $E_i$ of $N$-electron atomic Hamiltonian $H$ is addressed to the solution of eigenvalue equations $H_{\text{eff}}\Phi(i) = E_i\Phi(i)$, where the model functions $\Phi(i)$ are determined in Eq. (6). However, in practical applications, the accuracy of effective Hamiltonian $H_{\text{eff}}$ is finite. In this section, we consider the third-order contribution to $H_{\text{eff}}$. 
The third-order approximation $H_{\text{eff}}^{(3)}$ is represented by Eq. (14), replacing $\hat{\Omega}_n$ with the second-order contribution $\hat{\Omega}^{(2)} = \sum_{n=1}^{4} \hat{\Omega}^{(2)}_n$. Then

$$H_{\text{eff}}^{(3)} = \sum_{m=1}^{2} \sum_{n=1}^{4} \min(2m,2n) \sum_{\xi=1}^{\text{min}(2m,2n)} \hat{h}^{(3)}_{mn;\xi}; \quad \hat{h}^{(3)}_{mn;\xi} = \{ \hat{P} V_m \hat{\Omega}^{(2)}_n \hat{P} \}_{\xi}. \quad (15)$$

The task under consideration is divided into two parts: (1) the determination of $\hat{\Omega}_n^{(2)}$ with $n = 1, 2, 3, 4$; (2) the construction of $\hat{h}^{(3)}_{mn;\xi}$ for $m + n - \xi = 1, 2$.

### A. The determination of terms of the second-order wave operator

In the first part, the operators $\hat{\Omega}_n^{(2)}$ are generated in accordance with Ref. 6 (Eq. (13.30), p. 302). The terms are computed by using the NCoperators package which is programmed upon Propositions [II.2][II.4] and Corollaries [II.5][II.6]. This part of computation is the most time consuming process. The generated terms are arranged by passing to Theorem [II.7]. The coefficients $\omega^{(2)}_{\alpha\beta}, \omega^{(2)}_{\alpha\beta\mu\nu}, \omega^{(2)}_{\alpha\beta\mu\nu\eta\theta}$ located next to the operators $\hat{O}_1, \hat{O}_2, \hat{O}_3$ and $\hat{O}_4$ in Eq. (15), are treated as the effective one-, two-, three- and four-particle matrix elements on the basis of the product of accordingly same number one-electron eigenstates $\varphi(n_\alpha \lambda_\alpha m_\alpha)$. Here $\lambda_\alpha$ denotes the irreducible representation of $G$ (Sec. [II.A]). The basis index acquires the values $m_\alpha = -\lambda_\alpha, -\lambda_\alpha + 1, \ldots, \lambda_\alpha - 1, \lambda_\alpha$. Then the Wigner-Eckart theorem is applied to each matrix element, and the basis indices are excluded to the Clebsch-Gordan coefficients of SU(2). Despite of a large number of matrix elements $\omega^{(2)}$, there are only a few of fundamental constructions to be examined; other elements are derived by varying the given ones. These SO(3)-invariant constructions are produced in Tabs. [III]. All computed effective matrix elements $\omega^{(2)}$, necessary to form one-body and two-body terms of the effective Hamiltonian, are presented in an explicit form in Appendix [A]. The analysis of these elements is performed in the next part of computation.

Let us study the structure $\sum_{\xi\bar{\mu}} v_{\xi\alpha\bar{\nu}} \bar{\nu}_{\alpha\xi\bar{\mu}}/(\varepsilon_{\xi\bar{\nu}} - \varepsilon_{\alpha\bar{\mu}})$ as an example. Here $\varepsilon_{\alpha\beta\ldots\zeta} = \varepsilon_\alpha + \varepsilon_\beta + \ldots + \varepsilon_\zeta$, where $\varepsilon_\alpha$ denotes the one-electron energy. The one-electron matrix element is given by $v_{\xi\alpha\bar{\mu}} = \langle \varphi(n_\zeta \lambda_\zeta m_\zeta) \cdot v_{\mu_1}^{\alpha_1} \varphi(n_\mu \lambda_\mu m_\mu) \rangle_{\beta} \equiv \langle n_\zeta \lambda_\zeta m_\zeta | v_{\mu_1}^{\alpha_1} | n_\mu \lambda_\mu m_\mu \rangle$. The operator $v$ acts on a single-particle Hilbert space $\mathcal{H}$. Hereafter, the irreducible representation $\tau_1$ labels the one-electron operator $v$ which befits to a second quantized form $V_1$ in the generalized Bloch equation, written for $\hat{\Omega}^{(2)}$; the one-electron operator $v$, located in $\hat{\Omega}^{(1)}$, will be labeled by $\tau_2$;
TABLE I. The multipliers for effective one-particle matrix elements of $\tilde{\Omega}^{(2)}$

| Element: Expression |
|---------------------|
| $(ii\xi)$ |

(111) $S_{\alpha\beta}(\tau_1\tau_2\tau)$ :

$$(-1)^{\lambda_3-\lambda_1-\tau} \sum_{\mu} \frac{f(\tau_1\lambda_\alpha\lambda_\mu)f(\tau_2\lambda_\mu\lambda_\beta)}{\varepsilon_\beta-\varepsilon_\mu} \{ \tau_1 \tau_2 \tau \}$

(122) $\tilde{S}_{\alpha\beta}(\tau_1)$ :

$$2(-1)^{\lambda_\alpha+\lambda_\beta} \sum_{\zeta\mu} \sum_{\rho\xi} \sum_{\xi_\rho\delta} \sum_{\mu_\rho} \{ (-1)^{\lambda_\rho-\lambda_\eta} \sum_{\xi_\rho\delta} \sum_{\mu_\rho} \{ \tau_1 \tau_2 \tau \}$

(212) $\tilde{S}'_{\alpha\beta}(\tau_2)$ :

$$\tilde{R}(\beta_\zeta\rightarrow\mu)\tilde{S}_{\alpha\beta}(\tau_2)$$

(223) $\tilde{S}_{\alpha\beta}$ :

$$4\delta_{\alpha\beta}\lambda_\beta|\lambda_\alpha|^{-1/2} \sum_{\rho\xi} \sum_{\xi_\rho\delta} \sum_{\mu_\rho} \{ (-1)^{\lambda_\rho-\lambda_\eta} \sum_{\xi_\rho\delta} \sum_{\mu_\rho} \{ \tau_1 \tau_2 \tau \}$

TABLE II. The multipliers for effective two-particle matrix elements of $\hat{\Omega}^{(2)}$

| Element: Expression |
|---------------------|
| $(ii\xi)$ |

(110) $D_{\alpha\beta\mu\nu}(ud\tau)$ :

$$[\tau_1, \tau_2, u, d]^{1/2} \sum_{\xi, \eta} \frac{f(\tau_1\lambda_\alpha\lambda_\eta)f(\tau_2\lambda_\eta\lambda_\mu)}{\varepsilon_\eta-\varepsilon_\xi} \{ \tau_1 \tau_2 \tau \}$

(121) $D_{\alpha\beta\mu\nu}(Uu\tau_1)$ :

$$2(-1)^{\lambda_\alpha+\lambda_\beta} \sum_{\zeta\mu} \sum_{\rho\xi} \sum_{\xi_\rho\delta} \sum_{\mu_\rho} \{ \tau_1 \tau_2 \tau \}$

(211) $D'_{\alpha\beta\mu\nu}(Uu\tau_2)$ :

$$\tilde{R}(\beta_\zeta\rightarrow\alpha)D_{\alpha\beta\mu\nu}(Uu\tau_2)$$

(222) $D_{\alpha\beta\mu\nu}(uu)$ :

$$4(-1)^{\lambda_\mu+\lambda_\nu+i\xi}[u]^{-1/2} \sum_{\zeta\rho} \sum_{\rho\xi} \sum_{\xi_\rho\delta} \sum_{\mu_\rho} \{ \tau_1 \tau_2 \tau \}$

(222) $\Delta_{\alpha\beta\mu\nu}(UU)$ :

$$4(-1)^{U-\lambda_\mu} \sum_{\xi, \eta} \sum_{\zeta\rho} \sum_{\rho\xi} \sum_{\xi_\rho\delta} \sum_{\mu_\rho} \{ \tau_1 \tau_2 \tau \}$$
TABLE III. The multipliers for effective three- and four-particle matrix elements of $\tilde{\Omega}^{(2)}$

| $(ij\xi)$ Element: Expression |
|--------------------------------|
| $(120)$ $T_{\alpha\beta\zeta\mu\rho\eta}(u_1)$ : |
| $2(-1)^{\lambda\zeta\alpha+\lambda\eta+u}f(\tau_1\lambda_\alpha\lambda_\eta)\epsilon(0\lambda_\beta\lambda_\eta\lambda_\rho uu)$ |
| $(210)$ $T_{\alpha\beta\zeta\mu\rho\eta}(u_2)$ : |
| $\tilde{R}(\epsilon_{\alpha\beta\zeta\rho\eta}) T_{\alpha\beta\zeta\mu\rho\eta}(1) \tau_2$ |
| $(221)$ $(-1)^M T_{\alpha\beta\zeta\mu\rho\eta}(DdU) :$ |
| $4(1)^{\lambda\eta-\lambda\rho+\lambda\delta+\lambda\theta}z(0\lambda_\alpha\lambda_\beta\lambda_\rho\lambda_\mu uu)$ |
| $(220)$ $Q_{\alpha\beta\zeta\mu\rho\eta}(u_d)$ : |
| $\left[12\right] u^{d+\lambda_\mu+\lambda_\delta+\lambda_\rho+\lambda_\eta} z(0\lambda_\alpha\lambda_\beta\lambda_\rho\lambda_\mu uu) z(0\lambda_\xi\lambda_\beta\lambda_\delta\lambda_\eta dd)$ |

The operator $v$ in $V_1$ of Eq. (15) will be labeled by $\tau_0$. We assume that $v_{mn1}^{(1)} = (-1)^{\Xi(\tau_1 m_1)} v_{mn1}^{(1)}$ and $v_{\zeta\mu} = v_{\bar{\mu}\zeta}$. This implies

$$f(\tau_1\lambda_\mu\lambda_\zeta) = \epsilon(\tau_1\lambda_\zeta\lambda_\mu)f(\tau_1\lambda_\zeta\lambda_\mu),$$  \hspace{1cm} (16)

$$\epsilon(\tau_1\lambda_\zeta\lambda_\mu) = (-1)^{\lambda_\zeta-\lambda_\mu}[\tau_1]^{-1} \sum_{m_1 = -\tau_1}^{+\tau_1} (-1)^{m_1 - \tau(\tau_1 m_1)},$$  \hspace{1cm} (17)

$$f(\tau_1\lambda_\zeta\lambda_\mu) = -\left[\lambda_\zeta\right]^{1/2}[\tau_1]^{-1} \frac{n_\zeta\lambda_\zeta||v_{\tau_1}||n_\mu\lambda_\mu],$$  \hspace{1cm} (18)

where $[x] \equiv 2x + 1$. The phase multiplier $\Xi$ is optional. Usually it is chosen to be equal to $15$ $\Xi(\tau_1 m_1) = \tau_1 - m_1$. Then $\epsilon(\tau_1\lambda_\zeta\lambda_\mu) = (-1)^{\lambda_\zeta-\lambda_\mu+\tau_1}$. Particularly, if $v_k^q = rC^k_q$ represents the multipole momentum, then $f(kl_\mu l_\zeta) = f(kl_\zeta l_\mu)$, since $\lambda_\zeta, l_\zeta = l_\zeta, l_\zeta^\mu$ and the reduced matrix element $[\zeta||C^k||\mu] \neq 0$, if $l_\zeta + l_\mu + k$ is even. The state $\phi(\lambda_\alpha\lambda_\alpha m_\alpha)$ denotes either 2-spinor or 4-spinor, thus Eqs. (16)-(18) hold for both – none relativistic and relativistic – approaches. We assume that the one-electron Slater integrals are involved in the definition of $f$. The two-particle-matrix element with tilde equals to $\tilde{v}_{\mu \alpha \zeta \bar{\beta}} = v_{\mu \alpha \zeta \bar{\beta}} - v_{\mu \alpha \bar{\beta} \zeta}$, where the element $v_{\mu \alpha \zeta \bar{\beta}} = \langle n_\mu \lambda_\mu m_\mu n_\alpha \lambda_\alpha m_\alpha | g_{\tau_1}^\gamma | n_\zeta \lambda_\zeta m_\zeta n_\beta \lambda_\beta m_\beta \rangle$. In general, the two-particle interaction operator $g_{12}$ acts on $\mathcal{F} \times \mathcal{F}$. However, $g^\gamma$ is reduced and it acts on irreducible tensor space $\mathcal{F}^\gamma$, obtained by reducing (Sec. 2, Eq. (3)) $\mathcal{F}^{\gamma_1} \times \mathcal{F}^{\gamma_2}$. We also account for only scalar representations $\gamma = 0$, and self-adjoint operators $g_{12}^\dagger = g_{12}$. This implies...
TABLE IV. The expansion coefficients for one-body terms of the third-order contribution to the effective Hamiltonian

\[
\langle mn\xi\rangle \mathfrak{h}^{(3)+}_{mn\xi}(\Lambda) \tag{111}
\]

\[
(-1)^{l_0-l_v} [\tau_0]^{1/2} \sum_{\alpha=\nu,\epsilon} \langle \tau_0 m_0 \alpha M|\Delta M \rangle \left( (-1)^{l_\lambda} \sum_{e} f(\tau_0 \lambda_\nu \lambda_\epsilon) \Omega^{(2)+}_{\epsilon\nu}(\Lambda) \right) \left\{ \begin{array}{ccc} \tau_0 & \alpha & \Lambda \\ \lambda_\nu & \lambda_\epsilon & \lambda_\lambda \end{array} \right\} \\
-(-1)^{l_\lambda} \sum_{e} f(\tau_0 \lambda_\nu \lambda_\epsilon) \Omega^{(2)+}_{e\nu}(\Lambda) \left\{ \begin{array}{ccc} \tau_0 & \epsilon & \Lambda \\ \lambda_\nu & \lambda_\epsilon & \lambda_\lambda \end{array} \right\}
\]

\[
2(-1)^{l_\nu-l_v} \sum_{\alpha=\nu,\epsilon} \langle \tau_0 m_0 \alpha M|\Delta M \rangle \sum_{e} \tilde{z}(0\lambda_\nu \lambda_\epsilon \lambda_\alpha \alpha \epsilon \epsilon \alpha) \Omega^{(2)+}_{\epsilon\nu}(\Lambda)[u]^{1/2} \left\{ \begin{array}{ccc} \lambda_\nu & \lambda_\epsilon & \lambda_\lambda \\ u & \lambda_\alpha & \lambda_\lambda \end{array} \right\} \tag{121}
\]

\[
(-1)^{l_\lambda} [\tau_0]^{1/2} \sum_{A_1 A_2 \overline{A}} (-1)^{l_\lambda} [A_1, A_2, \overline{A}]^{1/2} \langle \tau_0 m_0 \lambda_\mu \lambda_\lambda |\Delta M \rangle \sum_{c} \left( \sum_{e} (-1)^{l_\lambda-\lambda_\nu} f(\tau_0 \lambda_\nu \lambda_\nu) \right) \times \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\mu & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\nu & \lambda_\lambda \end{array} \right\} \\
2 \sum_{A_1 A_2} [A_1]^{1/2} \sum_{c} \left( a(\lambda_\nu \lambda_\lambda \Lambda) \sum_{e} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\alpha \lambda_\epsilon \lambda_\alpha) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} A_1 & A_2 & \Lambda \\ \lambda_\nu & \lambda_\nu & \lambda_\lambda \end{array} \right\} \\
- \sum_{e} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\lambda \lambda_\alpha \lambda_\epsilon \lambda_\alpha) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\nu & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\lambda & \lambda_\lambda \end{array} \right\} \right) + 2 \sum_{A_1 A_2} (-1)^{l_\lambda} [A_2]^{1/2}
\]

\[
2 \sum_{e} \sum_{\alpha=\nu,\epsilon} \sum_{A_1 A_2} a(\lambda_\nu \lambda_\lambda \Lambda) \sum_{e} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\alpha \lambda_\epsilon \lambda_\alpha) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\lambda & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\nu & \lambda_\lambda \end{array} \right\} + \sum_{A_1 A_2 \overline{A}} (-1)^{l_\lambda+\lambda_\nu+\lambda_\nu} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\lambda \lambda_\alpha \lambda_\epsilon \lambda_\alpha) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\lambda & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\nu & \lambda_\lambda \end{array} \right\} \\
+a(\lambda_\lambda \lambda_\nu \lambda_\lambda) \sum_{\mu-\nu-\mu} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\nu \lambda_\nu \lambda_\nu) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\lambda & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\nu & \lambda_\lambda \end{array} \right\}
\]

\[
2 \sum_{c} \sum_{\epsilon=\nu,\nu} \sum_{\alpha=\nu,\epsilon} \sum_{A_1 A_2} a(\lambda_\nu \lambda_\lambda \Lambda) \sum_{e} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\alpha \lambda_\epsilon \lambda_\alpha) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\lambda & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\nu & \lambda_\lambda \end{array} \right\} + \sum_{A_1 A_2 \overline{A}} (-1)^{l_\lambda+\lambda_\nu+\lambda_\nu} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\nu \lambda_\nu \lambda_\nu) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\lambda & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\nu & \lambda_\lambda \end{array} \right\} \\
+a(\lambda_\lambda \lambda_\nu \lambda_\lambda) \sum_{\mu-\nu-\mu} \tilde{z}(0\lambda_\lambda \lambda_\epsilon \lambda_\nu \lambda_\nu \lambda_\nu) \Omega^{(2)+}_{\epsilon\mu}(\Lambda) \left\{ \begin{array}{ccc} \lambda_\lambda & \lambda_\nu & \lambda_\lambda \\ \lambda_\lambda & \lambda_\nu & \lambda_\lambda \end{array} \right\}
\]

\[v_{\mu_\alpha_\zeta_{\beta}} = v_{\alpha_\beta_\mu_\zeta} = v_{\beta_\zeta_\alpha_\mu}. \text{ In Ref.}^{25} \text{, it was showed that } v_{\mu_\alpha_\zeta_{\beta}} \text{ may be constructed in two distinct ways: (i) reducing the Kronecker product } (\lambda_\mu \times \lambda_\zeta) \times (\lambda_\alpha \times \lambda_\beta) \text{ (b-scheme); (ii) }\]

\[\text{reducing the Kronecker product } (\lambda_\mu \times \lambda_\alpha) \times (\lambda_\zeta \times \lambda_\beta) \text{ (z-scheme). Then the two-particle reduced matrix element is formed in terms of either } b(0\lambda_\mu \lambda_\alpha \lambda_\beta \lambda_\zeta \gamma_1 \gamma_1) \text{ or } z(0\lambda_\mu \lambda_\alpha \lambda_\beta \lambda_\zeta \Gamma_1 \Gamma_1) \text{ coefficient}^{25} \text{ (Sec. 2, Eqs. (24), (30)) for } \gamma = 0. \]

\[\text{Usually the authors (see above cited works) better prefer b-scheme, as it is more convenient to produce the algebraic expression, written for a particular Goldstone diagram. Then a two-particle matrix element is denoted } v_{\mu_\alpha_\zeta_{\beta}} \equiv g_{\mu_\alpha_\zeta_{\beta}} \text{ and } \tilde{v}_{\mu_\alpha_\zeta_{\beta}} \equiv \tilde{g}_{\mu_\alpha_\zeta_{\beta}}; \text{ the correspondent reduced matrix elements are given by } X_{\mu_\alpha_\zeta_{\beta}} \text{ and } Z_{\mu_\alpha_\zeta_{\beta}} \text{ (see, for example, Ref.}^{2}\]

\[13\]
(Appendix, Eqs. (A1), (A5)). Contrarily, in this paper we give priority exceptionally to the algebraic analysis of terms, and, along with Theorem 11.7, the z-scheme is more preferable for the arrangement of their irreducible tensor form. Then \( v_{\rho \alpha \zeta \tilde{\beta}} (\tilde{v}_{\rho \alpha \zeta \tilde{\beta}}) \) will be expressed by \( z(0\lambda_\mu \lambda_\alpha \lambda_\beta \lambda_\zeta \Gamma_1 \Gamma_1) \) \( (\tilde{z}(0\lambda_\mu \lambda_\alpha \lambda_\beta \lambda_\zeta \Gamma_1 \Gamma_1)) \), where

\[
\tilde{z}(0\lambda_\mu \lambda_\alpha \lambda_\beta \lambda_\zeta \Gamma_1 \Gamma_1) = z(0\lambda_\mu \lambda_\alpha \lambda_\beta \lambda_\zeta \Gamma_1 \Gamma_1) - a(\lambda_\zeta \lambda_\beta \Gamma_1) z(0\lambda_\mu \lambda_\alpha \lambda_\zeta \lambda_\beta \Gamma_1 \Gamma_1),
\]

where \( a(\lambda_\zeta \lambda_\beta \Gamma_1) = (-1)^{\lambda_\zeta + \lambda_\beta + \Gamma_1} \). The studied effective one-particle matrix element is represented by

\[
\sum_{\zeta \mu} v_{\zeta \mu} \tilde{v}_{\mu \alpha \zeta \tilde{\beta}} = (-1)^{\lambda_\beta + m_\beta} \tilde{S}_{\alpha \beta}(\tau_1) \langle \lambda_\alpha m_\alpha \lambda_\beta - m_\beta | \tau_1 m_1 \rangle,
\]

where \( \tilde{S}_{\alpha \beta}(\tau_1) \) plays a role of the effective one-particle reduced matrix element. The quantity \( \langle \lambda_\alpha m_\alpha \lambda_\beta - m_\beta | \tau_1 m_1 \rangle \) denotes the Clebsch-Gordan coefficient of SU(2). Moreover, the form of Eq. (20) directly indicates that the one-particle operator, given by the product of \( \hat{O}_1 = a_\alpha a_\beta^\dagger \) and Eq. (20), is simply equal to \( W^{\tau_1}_m(\lambda_\alpha \lambda_\beta) \tilde{S}_{\alpha \beta}(\tau_1) \), where the irreducible tensor operator \( W^{\tau_1}(\lambda_\alpha \lambda_\beta) = [a^{\lambda_\alpha} \times \bar{a}^{\lambda_\beta}]^{\tau_1} \) is obtained by reducing \( \hat{O}_1 \). The representation \( \lambda_\beta \) designates the transposed annihilation operator \( \bar{a}_{m_\beta}^{\lambda_\beta} = (-1)^{\lambda_\beta - m_\beta} a_{-m_\beta}^{\lambda_\beta} \). The matrix elements of \( W^{\tau_1} \) can be found in Refs. 20, 27. Here and elsewhere, it is considered if necessary that the summation is fulfilled over all given one-electron orbitals of marked type. However, only the sum running over the repetitive orbitals (\( \zeta, \bar{\mu} \) in this case) will be written.

In Tabs. the index \( i = 1, 2 \) labels \( V_i \), while \( j = 1, 2 \) labels \( \Omega_j^{(1)} \). The operator \( \hat{R} \) replaces orbitals in denominators. For example, the expression \( \hat{R}^{\rho \eta \bar{\mu}}_{\beta \zeta \alpha} (\varepsilon_{\eta \bar{\mu}} - \varepsilon_{\beta \zeta})^{-1} \) reads \( (\varepsilon_{\bar{\mu}} - \varepsilon_{\alpha})^{-1} \). The quantities \( \{ j_1^{l_1} j_2^{l_2} j_3^{l_3} \} \) and \( \{ j_1^{l_1} j_2^{l_2} j_3^{l_3} \} \) denote 6j- and 9j-symbols. The elements which are found by making the three-pair contractions between \( V_2 \) and \( \Omega_2^{(1)} \) vanish, if representations \( \lambda_\alpha \neq \lambda_\beta \) in \( W^{0}(\lambda_\alpha \lambda_\beta) \). In this case, the orbitals \( \zeta, \rho, \eta \) are identical for all \( \alpha, \beta \): \( \zeta = \rho = \eta = V \). Also, we mark off \( K_{\alpha \beta} \equiv \tilde{S}_{\alpha \beta}, \tilde{S}'_{\alpha \beta} \) by the summation parameter \( \mu \equiv n_\mu \mu_\mu \): (i) if \( \mu = V \), then \( K_{\alpha \beta} = \bar{K}_{\alpha \beta} \); (ii) if \( \mu = e \), then \( K_{\alpha \beta} = \bar{K}_{\alpha \beta} \); (iii) if \( \mu = c \), then we simply write \( K_{\alpha \beta} \). The tildes designate that the direct and exchanged parts of a two-particle matrix element are involved. If given \( D_{\alpha \beta \bar{\mu} \bar{\rho}}(\bar{U} u \tau_1) \), then \( \bar{U} \) marks \( \bar{v} \), represented by \( V_2 \). Additionally, if given \( D_{\alpha \beta \bar{\mu} \bar{\rho}}(U \bar{u} \tau_1) \), then \( \bar{u} \) marks \( \bar{v} \), fitted to \( \Omega_2^{(1)} \). For both \( \bar{U} \) and \( \bar{u} \), we write \( \bar{D}_{\alpha \beta \bar{\mu} \bar{\rho}}(U u \tau_1) \). A similar argument holds for the rest of elements in Tabs. These elements are also separated by the summation parameters. If \( \xi = 1 \),
TABLE V. The expansion coefficients for two-body terms of the third-order contribution to the effective Hamiltonian

\[
(mn\xi) \Theta_{mn\xi}^{(3)}(\Lambda_1\Lambda_2\Lambda)
\]

\[
-\left[\tau_0\right]^{-1/2} \sum_\lambda \left(\frac{\Lambda_1}{\lambda} - \frac{\bar{\Lambda}_1}{\bar{\lambda}}\right) \left(-1\right)^{\lambda_0} a(\lambda_\nu\lambda_\eta, \tau_0) a(\Lambda_1\Lambda_2\Lambda)[\Lambda_1]^{1/2} \langle\tau_0 m_0 \bar{\Lambda}_1 \bar{\Lambda}_2 \bar{\Lambda} | \Delta M | \Lambda_1 \Lambda_2 \Lambda\rangle \left\{\begin{array}{c}
\tau_0 \frac{\Lambda_1}{\lambda} \\
\Lambda_2 \bar{\lambda}
\end{array}\right\}
\times \sum_e f(\tau_0 \lambda_\nu \lambda_\eta) \Omega_e^{(2)+} \left(\Lambda_1 \Lambda_2 \Lambda\right) \left\{\begin{array}{c}
\tau_0 \lambda_\nu \\
\lambda_\eta
\end{array}\right\} + (-1)^{m_0} a(\Lambda_1\Lambda_2\Lambda)[\Lambda_2]^{1/2} \langle\tau_0 - m_0 \bar{\Lambda}_1 \bar{\Lambda}_2 \bar{\Lambda} | \Delta M | \Lambda_1 \Lambda_2 \Lambda\rangle
\times \left\{\begin{array}{c}
\tau_0 \frac{\Lambda_2}{\lambda} \\
\Lambda_1 \bar{\lambda}
\end{array}\right\} \sum_c f(\tau_0 \lambda_\nu \lambda_\eta) \Omega_c^{(2)+} \left(\Lambda_1 \Lambda_2 \Lambda\right) \left\{\begin{array}{c}
\tau_0 \lambda_\nu \\
\lambda_\eta
\end{array}\right\}
\]

\[
(-1)^{\lambda_\nu + \Lambda} \left[A_2\right]^{1/2} \sum_e (-1)^{\lambda_\nu} \bar{Z}(\lambda_\nu, \lambda_\eta, \lambda_\eta, \lambda_1 \Lambda_1) \Omega_e^{(2)+} (\Lambda_1 \Lambda_2 \Lambda) \left\{\begin{array}{c}
\Lambda_1 \\
\Lambda_2 \\
\Lambda
\end{array}\right\} - (-1)^{\lambda_\nu + \Lambda_1} \left[A_1\right]^{-1/2}
\times \sum_c \bar{Z}(\lambda_\nu, \lambda_\eta, \lambda_\eta, \lambda_1 \Lambda_1) \Omega_c^{(2)+} (\Lambda_1 \Lambda_2 \Lambda) \left\{\begin{array}{c}
\Lambda_1 \\
\Lambda_2 \\
\Lambda
\end{array}\right\}
\]

\[
a(\lambda_\nu \lambda_\eta \Lambda_2)[\Lambda_1]^2 \sum_e \bar{Z}(\lambda_\nu \lambda_\eta, \lambda_1 \Lambda_1) \Omega_e^{(2)+} (\Lambda_1 \Lambda_2 \Lambda) + (-1)^{\lambda_\nu + \lambda_1 \Lambda_1}
\times \sum_e \sum_{\mu=v,e} \bar{Z}(\lambda_\nu \lambda_\eta, \lambda_1 \Lambda_1) \Omega_e^{(2)+} (\Lambda_1 \Lambda_2 \Lambda) + 2(-1)^{\Lambda_1 + \Lambda_2} \left[A_1, \Lambda_2\right]^{1/2} \sum_{\bar{\Lambda}_1 \bar{\Lambda}_2 \bar{\Lambda}} \bar{Z}(\lambda_\nu \lambda_\eta, \lambda_1 \Lambda_1) \Omega_e^{(2)+} (\Lambda_1 \Lambda_2 \Lambda) \left\{\begin{array}{c}
\Lambda_1 \\
\Lambda_2 \\
\Lambda
\end{array}\right\}
\]

\[
(-1)^{\lambda_\nu + \lambda_1 \Lambda_1} \sum_{c' \mu} (-1)^{\lambda_\nu + \lambda_1 \Lambda_1} \bar{Z}(\lambda_\nu \lambda_\eta, \lambda_1 \Lambda_1) \Omega_{c'}^{(2)+} (\Lambda_1 \Lambda_2 \Lambda) \left\{\begin{array}{c}
\Lambda_1 \\
\Lambda_2 \\
\Lambda
\end{array}\right\}
\]

\[
(1)_{\sigma}^{1/2} \sum_{\mu=v,e} \sum_{\bar{\Lambda}_2 \bar{\Lambda}_3 \bar{\Lambda}_4} \left(-1\right)\bar{Z}(\lambda_\nu \lambda_\eta, \lambda_1 \Lambda_1) \Omega_{c'}^{(2)+} (\Lambda_1 \Lambda_2 \Lambda) \left\{\begin{array}{c}
\lambda_\nu \\
\lambda_\eta \\
\lambda_1 \\
\lambda_2 \\
\lambda_3 \\
\lambda_4
\end{array}\right\}
\times \left\{\begin{array}{c}
\Lambda_1 \\
\Lambda_2 \\
\Lambda_3 \\
\Lambda_4
\end{array}\right\}
\times \left\{\begin{array}{c}
\lambda_\nu \\
\lambda_\eta \\
\lambda_1 \\
\lambda_2 \\
\lambda_3 \\
\lambda_4
\end{array}\right\}
\times \left\{\begin{array}{c}
\lambda_\nu \\
\lambda_\eta \\
\lambda_1 \\
\lambda_2 \\
\lambda_3 \\
\lambda_4
\end{array}\right\}
\]

267 then the notations are similar to \(K_{\alpha \beta}\) case. If \(\xi = 2\) (see Tab. ||), then for \(D_{\alpha \beta \rho}(uu)\), we write: (i) if \(\zeta, \rho = c\), then \(D = D\); (ii) if \(\zeta, \rho = v\), then \(D = \bar{D}\); (iii) if \(\zeta, \rho = e\), then \(D = \bar{D}\); (iv) if \(\zeta = e\) and \(\rho = v\), then \(D = \bar{D}\). For \(\zeta = v\) and \(\rho = e\), the similar triple doted \(\bar{D}\) is considered. This is due to the symmetry properties of \(v_{\alpha \beta \rho}\). Finally, for \(\Delta_{\alpha \beta \rho}(UU)\), we write: (i) if \(\rho = v\), then \(\Delta = \bar{\Delta}\); (ii) if \(\rho = e\), then \(\Delta = \bar{\Delta}\). In these cases, \(\zeta = c\).
The determination of terms of the third-order effective Hamiltonian

By Proposition II.2 it follows that this part of computation requires significantly less time than the first one. Besides, the none zero terms of \( \hat{h}_{mn;\xi}^{(3)} \) are derived in accordance with Theorem II.7 which allows to reject a large amount of \( \hat{\Omega}^{(2)} \) terms, attaching the zero-valued contributions. The operators \( \hat{h}_{mn;\xi}^{(3)} \) are considered by the formulas

\[
\hat{h}_{mn;\xi}^{(3)} = \sum_{\Lambda M} W^\Lambda_M (\lambda_v \tilde{\lambda}_{v'}) h_{mn;\xi}^{(3)} (\Lambda),
\]

for \( m + n - \xi = 1 \), and

\[
\hat{h}_{mn;\xi}^{(3)} = -\sum_{\Lambda_1 \Lambda_2 \Lambda M} [W^{\Lambda_1}(\lambda_v \lambda_{v'}) \times W^{\Lambda_2}(\tilde{\lambda}_{v'} \tilde{\lambda}_{v})] \Lambda M h_{mn;\xi}^{(3)} (\Lambda_1 \Lambda_2 \Lambda),
\]

for \( m + n - \xi = 2 \). Each coefficient \( h_{mn;\xi}^{(3)} \) is additionally expressed by the sum of \( h_{mn;\xi}^{(3)+} \) and \( h_{mn;\xi}^{(3)-} \). The coefficients \( h_{mn;\xi}^{(3)+} \) are presented in an explicit form in Tabs. IV, V, VI. The coefficients \( h_{mn;\xi}^{(3)-} \) are derived from \( h_{mn;\xi}^{(3)+} \) by making the following alterations:

(a) \( \Omega_{\alpha\beta}^{(2)+}(\Lambda) \rightarrow (-1)^{L_{\alpha\beta} + M + 1} \Omega_{\alpha\beta}^{(2)-}(\Lambda); \)

(b) \( \Omega_{\alpha\beta\mu\nu}(\Lambda_1 \Lambda_2 \Lambda) \rightarrow (-1)^{L_{\alpha\beta\mu\nu} + M} \Omega_{\alpha\beta\mu\nu}^{(2)-}(\Lambda_1 \Lambda_2 \Lambda); \)

(c) \( \Omega_{\alpha\beta\gamma\delta\mu\nu}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda) \rightarrow (-1)^{L_{\alpha\beta\gamma\delta\mu\nu} + M + M_3 + 1} \Omega_{\alpha\beta\gamma\delta\mu\nu}^{(2)-}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda). \)

Here \( L_{\alpha\beta\ldots\gamma} = \lambda_{\alpha} + \lambda_{\beta} + \ldots + \lambda_{\gamma} \). In addition, there holds one more rule: (d) each basis index (if such exists) in \( h_{mn;\xi}^{(3)+} \), except for \( m_0 \), is replaced by the opposite sign index. In (a)-(c), the indices \( M \) and \( M_3 \) enumerate the basis for \( \Lambda \) and \( \Lambda_3 \), respectively. The quantities \( \Omega^{(2)+} \) are given in Appendix [A] while

\[
\tilde{\Omega}_{\alpha\beta\mu\nu}^{(2)+}(\Lambda_1 \Lambda_2 \Lambda) = \Omega_{\alpha\beta\mu\nu}^{(2)+}(\Lambda_1 \Lambda_2 \Lambda) - a(\lambda_\alpha \lambda_\beta \Lambda_1) \Omega_{\beta\mu\nu}^{(2)+}(\Lambda_1 \Lambda_2 \Lambda).
\]

Particularly, the \( \Omega^{(2)-} \) are derived by replacing the one-particle and two-particle matrix elements \( v_{\alpha\beta} \) and \( v_{\alpha\beta\mu\nu} \) with \( v_{\beta\alpha} \) and \( v_{\mu\alpha\beta} \) in order to obtain the standard form of the constructions that lay out in Tabs. II, III. For example, the element \( S_{\alpha\beta}(\tau_1 \tau_2 \tau) \) (Tab. I) is recognized from \( \sum_\mu v_{\alpha\mu} v_{\mu\beta}/(\varepsilon_\beta - \varepsilon_\mu) \) by excluding the SO(3)-invariant part. Thus, for \( \alpha = v, \beta = c, \mu = e, \) we get \( \tilde{S}_{vc}(\tau_1 \tau_2 \tau) \) which fits the definition of one-particle operator.
TABLE VI. The expansion coefficients for two-body terms of the third-order contribution to the effective Hamiltonian (continued)

\[ (mnξ)^{(3)+}_m (Λ_1 Λ_2 Λ) \]

\[
2[Λ_2]^{1/2} \sum_c (1-\lambda_c) \sum_\pi \pi_2 \pi_3 \pi (-1)^{\overline{3} \overline{2}(Λ_3, Λ)}^{1/2} \left( (1-\lambda_3) \overline{M} (M, Λ) \sum_c (\overline{m_1, Λ_1})^{1/2} \right) \\
\times (1-\lambda_\alpha') \overline{\zeta}(0, \lambda_\alpha' c, \lambda_\alpha', \lambda_\alpha', \lambda_\beta' \alpha' \zeta(2, Λ_2 Λ_2)) \{ δ_{\mu' ν'} \overline{M} (\mu', ν', Λ_2 Λ_2) \} \left( \sum_{\lambda_\alpha' \lambda_\alpha'} \right) \left( \bar{\lambda}_3 \bar{\lambda}_3 \bar{\lambda}_3 \right)

\[ \times \Omega^{(2)+}_μ ν' μ' ν' ν' c c' c (\bar{Λ}_1 \bar{Λ}_2 Λ_3 Λ_3) \left( \begin{array}{cccc}
\lambda_3 & \lambda_3 & \lambda_3 & \lambda_3 \\
\lambda_3 & \lambda_3 & \lambda_3 & \lambda_3 \\
\lambda_3 & \lambda_3 & \lambda_3 & \lambda_3 \\
\lambda_3 & \lambda_3 & \lambda_3 & \lambda_3 \\
\end{array} \right) - \delta_{\alpha_1, \alpha_1} (1-\lambda_\alpha' + \lambda_1)

\times (1-\lambda_\alpha') \zeta(0, \lambda_\alpha' c, \lambda_\alpha', \lambda_\alpha', \lambda_\alpha' \alpha' \zeta(2, Λ_2 Λ_2)) \left( \begin{array}{cccc}
\lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' \\
\lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' \\
\lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' \\
\lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' & \lambda_\alpha' \\
\end{array} \right)

\times \Omega^{(2)+}_μ ν' μ' ν' ν' c c' c (\bar{Λ}_1 \bar{Λ}_2 Λ_3 Λ_3) \left( \begin{array}{cccc}
\mu' & \mu' & \mu' & \mu' \\
\mu' & \mu' & \mu' & \mu' \\
\mu' & \mu' & \mu' & \mu' \\
\mu' & \mu' & \mu' & \mu' \\
\end{array} \right)

(233)

\[
(1-\lambda_\alpha') \zeta(0, \lambda_\alpha' c, \lambda_\alpha', \lambda_\alpha', \lambda_\alpha' \alpha' \zeta(2, Λ_2 Λ_2)) \left( \begin{array}{cccc}
\mu' & \mu' & \mu' & \mu' \\
\mu' & \mu' & \mu' & \mu' \\
\mu' & \mu' & \mu' & \mu' \\
\mu' & \mu' & \mu' & \mu' \\
\end{array} \right)

(244)

along with \( W_m^\tau (\lambda_\alpha \bar{λ}_c) \). On the other hand, another one-particle matrix element could be obtained from \( \sum_\mu \nu_\alpha \nu_\beta / (\varepsilon_\mu - \varepsilon_\alpha) \). The last element must be written in a standard form \( (-1) \sum_\mu \nu_\beta \nu_\alpha / (\varepsilon_\alpha - \varepsilon_\mu) \) to arrange the element \( S_\beta_\alpha (τ_1 τ_2 τ) \) correctly. For concrete values \( \alpha = \nu \) and \( \beta = c \), the orbital \( \mu \) equals to \( c \) only (see Proposition II.4), and the element is
denoted \( S_{cv}(\tau_1 \tau_2 \tau) \). In a tensor formalism, we gain the opposite sign of the basis index \( m \) in \( W^{\tau}_m(\lambda, \bar{\lambda}) \).

The diagrammatic interpretation of \( \hat{h}_{mn;\xi}^{(3)} \) can be clarified as follows. The diagrams of the third-order effective Hamiltonian \( H_{\text{eff}}^{(3)} \), assembled in \( \hat{h}_{mn;\xi}^{(3)} \), are derived by contracting the perturbation \( V_m \) with \( \hat{\Omega}_{n}^{(2)} \), where \( \hat{\Omega}_{n}^{(2)} \) includes: (i) the folded diagrams; (ii) some diagrams, obtained by contracting the core orbitals in Wick’s series; (iii) the diagrams, acceded to the reflection of a number of diagrams in \( \hat{\Omega}_{n}^{(2)+} \) about a horizontal axis. Note, \( \Omega_{\alpha\beta\rho\mu\nu\eta\sigma} \equiv \Omega_{\alpha\beta\rho\mu\nu\eta\sigma}^{(2)} \), since it is obtained from the disconnected diagrams \( V^2 \hat{\Omega}_{1}^{(1)} \) (see Tab. III).

C. The estimation of terms

The evaluation of the number of computed one-body terms (Tab. IV) of \( H_{\text{eff}}^{(3)} \) is presented in Tab. VII, where \( d^\pm \) denotes the number of direct terms in \( \hat{h}_{mn;\xi}^{(3)} \), while \( \bar{d}^\pm \) denotes the number of direct terms in \( \hat{h}_{mn;\xi}^{(3)} \), if the one-body interactions \( v^{\tau_i} \) \( (i = 0, 1, 2) \) are absent. Totally, there are computed \( 188 + 70 = 258 \) direct one-body terms of \( \hat{h}_{mn;\xi}^{(3)} \) and \( 72 + 20 = 92 \) direct one-body terms of \( \hat{h}_{mn;\xi}^{(3)} \), including the two-particle interactions \( g^0 \) only. For instance, Blundell et. al.\(^{17}\) calculated 84 diagrams contributing to the third-order mono-valent removal energy. In our considerations, their studied energies: a) \( E_A^{(3)} - E_H^{(3)} \); b) \( E_I^{(3)}, E_J^{(3)} \) and c) \( E_K^{(3)}, E_L^{(3)} \) (see Ref.\(^{17}\) (Sec. II, Eq. (8))) denote the matrix elements of terms in \( \hat{h}_{mn;\xi}^{(3)}, \hat{h}_{mn;\xi}^{(3)} \), \( \hat{h}_{mn;\xi}^{(3)} \) and \( \hat{h}_{mn;\xi}^{(3)} \), if \( g^0 \) represents the Coulomb interaction.

The estimation of the amount of two-body terms (Tabs. IV-VI) that contribute to \( H_{\text{eff}}^{(3)} \) is provided in Tab. VIII. There are \( 217 + 82 = 299 \) direct two-body terms in \( \hat{h}_{mn;\xi}^{(3)} \) and \( 125 + 42 = 167 \) direct two-body terms including the two-particle interactions \( g^0 \) only. In their study of beryllium and magnesium isoelectronic sequences, Ho et. al.\(^2\) calculated 218 two-body diagrams of the third-order perturbation. Analogous disposition to account for the two-particle interactions only, can be found in other works\(^{3,17,28}\). Additionally, most of them do not account for the folded diagrams.

Meanwhile, the expressions in Tabs. IV-VI obtained by exploiting the properties of proposed model space \( \mathcal{P} \) (Sec. III), have their own benefits:

1. The third-order contributions to the effective Hamiltonian \( H_{\text{eff}} \) are written in an operator form providing an opportunity to construct their matrix elements
TABLE VII. The amount of one-body terms in MBPT(3)

| (mnξ) | d⁺ | d⁺ | d⁻ | 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

efficiently. Namely, the irreducible tensor operators, labeled by the representations Λ (see Eqs. (21)-(22)), are written apart from the projection-independent parts. These angular coefficients include the structure coefficients Ω(2)±, multiplied by the 3nj-symbols. Particularly, the coefficients \( \{ j_1, j_2, j_3, j_4 \} \) and \( \{ k_1, k_2, k_3, k_4, k' \} \) (see Tabs. V-VI), denote the 12j-symbol of the first kind\( ^{(12)}j \) (Sec. 4-33, Eq. (33.17), p. 207) and the 15j-symbol of the third kind\( ^{(15)}j \) (Sec. 4-20, Eq. (20.3), p. 112).

2. The form of the expressions in Tabs. V-VI allows to evaluate the contributions of \( n \)-particle effects in CC approach. This is done by simply replacing \( \Omega(2)^± \) with \( \Omega_n \) (\( n = 1, 2, 3, 4 \)). By generally accepted labeling, such replacement leads to the transformation \( g_{\alpha\beta\ldots\zeta} \rightarrow \rho_{\alpha\beta\ldots\zeta} \), where \( \rho \) denotes the valence singles, doubles, triples, quadruples amplitude.

3. Obtained terms of the third-order perturbation include, in addition, the one-particle operators \( v^{\tau_i} (\tau_i = 0, 1, 2, \ldots) \) that represent the magnetic, hyperfine, etc. interactions. Moreover, the general expressions also fit none relativistic as well as the relativistic approaches. These effects are embodied in \( z(0\lambda_\alpha\lambda_\beta\lambda_\rho\lambda_\mu\Gamma_1\Gamma_1) \) coefficients.

4. The reduction scheme allows to write a large number of terms in a concise form. This feature becomes evident especially clearly when in contrast the terms are written side by side their diagrammatic representation.

Maintaining the completeness of the present discuss, we note that \( H_{\text{eff}}^{(3)} \) also includes the
TABLE VIII. The amount of two-body terms in MBPT(3)

| (mnξ) | d⁺ | d⁻ | d⁺ | 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 |

Terms \( \hat{h}^{(3)}_{mn;\xi} \) with \( m+n-\xi = 0, 3, 4, 5 \). For example, the coefficient \( \hat{h}^{(3)+}_{22;1} (E_1 \Lambda_1 E_2 \Lambda_2 \Lambda) \) reads

\[
\hat{h}^{(3)+}_{22;1} (E_1 \Lambda_1 E_2 \Lambda_2 \Lambda) = (-1)^{\lambda_\nu+\lambda_\psi+\lambda_\nu+\lambda_\psi+\Lambda_2+\Lambda}[\Lambda_1, \Lambda_2]^{1/2} \sum_{\Lambda_1} \sum_{\Lambda_2} a(\lambda_\nu, \lambda_\psi, \Lambda_2) \\
\times [E_1, E_2, \Lambda_1]^{1/2} \sum_{\nu\psi} \bar{z}(0 \lambda_\nu \lambda_\psi \lambda_\psi \lambda_\psi uu) \Omega^{(2)+}_{\nu\psi\psi\nu}(\Lambda_1 \Lambda_2 \Lambda) \\
\times \left\{ \lambda_\psi \Lambda_2 \Lambda_1 \right\} \left\{ \lambda_\nu \Lambda_2 \Lambda_1 \right\} \left\{ \lambda_\psi \Lambda_2 \Lambda_1 \right\} \left\{ \lambda_\psi \lambda_\psi \Lambda_2 \Lambda_1 \right\} \\
+ (-1)^{E_1+E_2} \sum_{\nu} \bar{z}(0 \lambda_\psi \lambda_\psi \lambda_\psi \lambda_\psi E_1 E_1) \Omega^{(2)+}_{\nu\psi\psi\nu}(\Lambda_1 \Lambda_2 \Lambda) \\
\times \left\{ \lambda_\nu \Lambda_1 \Lambda_1 \Lambda_1 \right\} \left\{ \lambda_\psi \Lambda_2 \Lambda_1 \Lambda_1 \right\} \left\{ \lambda_\psi \Lambda_2 \Lambda_1 \Lambda_1 \right\} \left\{ \lambda_\psi \Lambda_2 \Lambda_1 \Lambda_1 \right\}. \tag{24}
\]

This forms the three-body operator \( \hat{h}^{(3)}_{22;1} \) along with the irreducible tensor operator

\[
[[W^{E_1}(\lambda_\nu \lambda_\psi) \times a^{\lambda_\psi}]^{\Lambda_1} \times [W^{E_2}(\tilde{\lambda}_\psi \tilde{\lambda}_\psi) \times \tilde{a}^{\lambda_\psi}]^{\Lambda_2}]_{\Lambda_1}^{\Lambda_2}. \tag{25}
\]

However, the triple and higher-order effects are not covered by the examination of this paper.

IV. CONCLUSIONS

We present an algebraic technique to evaluate the terms of MBPT. The method relies on two main circumstances: the strictly determined operations of the Fock space operators on the vectors of the orthogonal subspaces of given separable Hilbert space, and the specific reduction scheme of terms of the PT. The aspiration to determine the behavior of the
Creation and annihilation operators is motivated by the fact that in higher-order perturbation theories, a huge number of terms is generated and, particularly, not all computed terms of the wave operator attach none zero contributions to the terms of effective interaction operator. Therefore the rules that allow to predetermine these valuable terms become meaningful. Meanwhile, in the PT, another no less important procedure is to work up the generated terms in order to calculate their matrix elements efficiently. If going on the traditional route, when each term is expressed side by side its diagrammatic representation, then once again one deals with the redundancy of terms and the procedure of reduction becomes troublesome. In this paper, however, we suggest the reduction scheme which is of versatile disposition. That is, the generated terms are combined in groups related to the different types of one-electron orbitals. Afterwards, we construct the effective matrix elements and apply the Wigner-Eckart theorem. In the result, we get the irreducible tensor operators and the projection-independent parts that are located apart from each other. This means the form of reduced terms becomes universal, only the SO(3)-invariant parts that embody the dynamics of studied physical interactions are changed. Since the method of reduction is applied to the third-order MBPT, we obtain maximum four-body effective matrix elements that are derived from the four-body parts of the second-order wave operator.

Finally, it is worth to mention that obtained symbolic preparation of terms of the MBPT(3) can be extremely simplified if applied to some special cases of interest. Mathematically, this means that some of the irreducible representations drawn in the $3nj$-symbols, in most cases would be simply equal to zero. Particularly, the $12j$- or $15j$-symbols would become the ordinary and widely used $6j$- or $9j$-symbols. Moreover, if the one-electron interactions, characterized by the none scalar representations, are not taken into account, then the irreducible one-body and two-body operators of the effective Hamiltonian are simply scalar operators. Thus their matrix elements become even simpler.
Appendix A: SO(3)-invariant part of the second-order wave operator

**One-body part.**

\( \Omega_{\mu e}^{(2)+}(\Lambda)(\varepsilon_e - \varepsilon_\mu) \)

\( = \delta_{\Lambda \tau} [\tilde{\mathcal{S}}_{\mu}(\tau_1 \tau_2 \tau) + \tilde{\mathcal{S}}_{\mu}(\tau_1 \tau_2 \tau)] + \delta_{\Lambda \tau_1} [\tilde{\mathcal{S}}_{\mu}(\tau_1) + \tilde{\mathcal{S}}_{\mu}(\tau_1)] 
+ \delta_{\Lambda \tau_2} [\tilde{\mathcal{S}}_{\mu}(\tau_2) + \tilde{\mathcal{S}}_{\mu}(\tau_2)] + \delta_{\Lambda 0} \tilde{\mathcal{S}}_{\mu}, \) \hfill (A1a)

\( \Omega_{\mu e}^{(2)-}(\Lambda)(\varepsilon_e - \varepsilon_\mu) = \delta_{\Lambda \tau} \tilde{S}_{\mu e}(\tau_1 \tau_2 \tau). \) \hfill (A1b)

**Two-body part.**

\( \Omega_{\mu'\mu''e}^{(2)+}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{ee'} - \varepsilon_{\mu'\mu''}) \)

\( = \delta_{\Lambda_1 \tau_1} \delta_{\Lambda_2 \tau_2} D_{\mu'\mu''e}(u_1 \tau_1) + \delta_{\Lambda_1 \tau_1} \delta_{\Lambda_2 \tau_2} [\mathcal{X}_{\mu'\mu''e'}(U_1 \tau_1) 
+ \mathcal{X}_{\mu'\mu''e'}(U_1 \tau_1)] + \delta_{\Lambda_1 \tau_1} \delta_{\Lambda_2 \tau_2} \mathcal{Z}_{\mu'\mu''e'}(U_1 \tau_2) 
\times \tilde{D}_{\mu'\mu''e'}(u_1 \tau_1) \) \hfill (A3a)

\( + \frac{1}{2} \mathcal{D}_{\mu'\mu''e'}(u_1 \tau_1) \) \hfill (A3b)

\( = -\frac{1}{2} \delta_{\Lambda_1 \tau_1} \delta_{\Lambda_2 \tau_2} \mathcal{Z}_{\mu'\mu''e'}(u_1 \tau_1) \tilde{D}_{\mu'\mu''e'}(u_1 \tau_1) 
+ \frac{1}{2} \delta_{\Lambda_1 \tau_1} \delta_{\Lambda_2 \tau_2} \mathcal{Z}_{\mu'\mu''e'}(u_1 \tau_2) \) \hfill (A3b)

\( + \mathcal{D}_{\mu'\mu''e'}(u_1 \tau_2) \) \hfill (A3b)

\( + \mathcal{D}_{\mu'\mu''e'}(u_1 \tau_2) \) \hfill (A3b)

\( + \mathcal{D}_{\mu'\mu''e'}(u_1 \tau_2) \) \hfill (A3b)

\( + \frac{1}{2} \delta_{\Lambda_1 \tau_1} \delta_{\Lambda_2 \tau_2} \mathcal{Z}_{\mu'\mu''e'}(u_1 \tau_2) D_{\mu'\mu''e'}(u_1 \tau_2). \) \hfill (A3b)
\( \Omega_{\text{evcc}}^{(2)^+}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{cc'} - \varepsilon_{ev}) \)

\[
= -\delta_{\Lambda_1} u \delta_{\Lambda_2} d \delta_{\Lambda \tau} Z_{\text{evcc}'}(u d \tau) D_{\text{evcc}'}(u d \tau) + \delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_1} \\
\times [\tilde{D}_{\text{evcc}'}(U u \tau_1) + Z_{\text{evcc}'}(U u \tau_1) \tilde{D}_{\text{evcc}'}(U u \tau_1)] \\
+ 4 \tilde{D}_{\text{evcc}'}(U u \tau_1) - \frac{1}{4} Z_{\text{evcc}'}(U u \tau_1) \tilde{D}_{\text{evcc}'}(U u \tau_1)]
\]

(A4a)

\( \Omega_{\text{evcc}}^{(2)^-}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{cc'} - \varepsilon_{ev}) \)

\[
= -\delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_1} Z_{\text{evcc}'}(u U \tau_1) \tilde{D}_{\text{evcc}'}(u U \tau_1) \\
+ \delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_2} Z_{\text{evcc}'}(u U \tau_2) [\tilde{D}'_{\text{evcc}'}(u U \tau_2) \\
+ \tilde{D}'_{\text{evcc}'}(u U \tau_2)].
\]

(A4b)

\( \Omega_{mu'ev}^{(2)^+}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{ev} - \varepsilon_{\mu' \mu''}) \)

\[
= \delta_{\Lambda_1} u \delta_{\Lambda_2} d \delta_{\Lambda \tau} \delta_{\mu' \mu''} [D_{ee' \sigma \phi}(u d \tau) - Z_{ee' \sigma \phi}(u d \tau) D_{ee' \sigma \phi}(u d \tau)] \\
+ \delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_1} [\tilde{D}_{\mu' \mu'' \phi}(U u \tau_1) - Z_{\mu' \mu'' \phi}(U u \tau_1) \\
\times \tilde{D}_{\mu' \mu'' \phi}(U u \tau_1)] + \delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_2} Z_{\mu' \mu'' \phi}(U u \tau_2) \tilde{D}'_{\mu' \mu'' \phi}(U u \tau_2) \\
+ \delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_0} [Z_{\mu' \mu'' \phi}(u) \{\tilde{\Delta}_{\mu' \mu'' \phi}(uu) + \tilde{\Delta}_{\mu' \mu'' \phi}(uu)\} \\
- \tilde{\Delta}_{\mu' \mu'' \phi}(uu) - \tilde{\Delta}_{\mu' \mu'' \phi}(uu) - 4 \tilde{D}_{\mu' \mu'' \phi}(uu),
\]

(A5a)

\( \Omega_{mu'ev}^{(2)^-}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{ev} - \varepsilon_{\mu' \mu''}) \)

\[
= -\delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_1} Z_{\text{evcc} \phi}(u U \tau_1) \{\tilde{D}_{\text{evcc} \phi}(u U \tau_1) \\
+ 4 \tilde{D}_{\text{evcc} \phi}(u U \tau_1)\} + Z_{\text{evcc} \phi}(u U \tau_1) D_{\text{evcc} \phi}(u U \tau_1)] \\
- \delta_{\Lambda_1} U \delta_{\Lambda_2} u \delta_{\Lambda \tau_2} [Z_{\text{evcc} \phi}(u U \tau_2) \{\tilde{D}'_{\text{evcc} \phi}(u U \tau_2) \\
+ \tilde{D}'_{\text{evcc} \phi}(u U \tau_2)] - Z_{\text{evcc} \phi}(u U \tau_2) \tilde{D}'_{\text{evcc} \phi}(u U \tau_2)].
\]

(A5b)
\[ \Omega^{(2)+}_{\text{evev}}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{\text{ev}} - \varepsilon_{\text{ev}}) \]

\[ = \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \left[ D^{\text{evev}}(u \tau_1) + Z_{\text{evev}}(u \tau_1) \right] \]

\[ + \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \left[ \tilde{D}^{\text{evev}}(u \tau_1) + \tilde{D}^{\text{evev}}(u \tau_1) - Z_{\text{evev}}(u \tau_1) \right] \]

\[ \times \{ \tilde{D}^{\text{evev}}(u \tau_1) + \tilde{D}^{\text{evev}}(u \tau_1) \} + \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \]

\[ \times \left[ - D^{\text{evev}}(u \tau_2) + Z_{\text{evev}}(u \tau_2) \tilde{D}^{\text{evev}}(u \tau_2) \right] \]

\[ - \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \left[ Z_{\text{evev}}(u \tau_2) \right] \]

\[ - \left[ \tilde{D}^{\text{evev}}(u \tau_2) + Z_{\text{evev}}(u \tau_2) \right] \tilde{D}^{\text{evev}}(u \tau_2) \]} \]

\[\Omega^{(2)-}_{\text{evev}}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{\text{ev}} - \varepsilon_{\text{ev}})\]

\[ = \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \left[ Z_{\text{evev}}(u \tau_1) \right] \]

\[ - \left[ \tilde{D}^{\text{evev}}(u \tau_1) + \tilde{D}^{\text{evev}}(u \tau_1) \right] \tilde{D}^{\text{evev}}(u \tau_1) \]

\[ \times \left\{ \tilde{D}^{\text{evev}}(u \tau_1) + \tilde{D}^{\text{evev}}(u \tau_1) \right\} + \frac{1}{2} \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \]

\[ \times \left[ Z_{\text{evev}}(u \tau_2) \tilde{D}^{\text{evev}}(u \tau_2) - \tilde{D}^{\text{evev}}(u \tau_2) \right] \]

\[ - \tilde{D}^{\text{evev}}(u \tau_2) + Z_{\text{evev}}(u \tau_2) \right\] \tilde{D}^{\text{evev}}(u \tau_2) \]

\[ - \tilde{D}^{\text{evev}}(u \tau_2) + Z_{\text{evev}}(u \tau_2) \right\} \tilde{D}^{\text{evev}}(u \tau_2) \]

\[\Omega^{(2)+}_{\text{evev}}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{\text{ev}} - \varepsilon_{\text{ev}})\]

\[ = - \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \left[ Z_{\text{evev}}(u \tau_1) \right] \tilde{D}^{\text{evev}}(u \tau_1) \]

\[ + \tilde{D}^{\text{evev}}(u \tau_1) \right\} \tilde{D}^{\text{evev}}(u \tau_1) \]

\[ + \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \left[ Z_{\text{evev}}(u \tau_2) \right] \tilde{D}^{\text{evev}}(u \tau_2) \]

\[ \times \tilde{D}^{\text{evev}}(u \tau_2) - \frac{1}{2} \delta_{\Lambda_1 U} \delta_{\Lambda_2 U} \delta_{\Lambda_1 U} \]

\[ \times \tilde{D}^{\text{evev}}(u \tau_2). \]
In Eq. (A3a), the quantities $X_{\mu'\mu''c'}$, $Y_{\mu'\mu''c'}$, $Z_{\mu'\mu''c'}$ differ for distinct one-electron orbitals $\mu = v, e$. If $\mu = v$, then $X_{vv'cc'} = \tilde{D}_{vv'cc'}$, $Y_{vv'cc'} = \tilde{D}_{vv'cc'}$ and $Z_{vv'cc'} = -Z_{vv'c'c}(u)D_{vv'c'c}$; if $\mu = e$, then $X_{ee'cc'} = \tilde{D}_{ee'cc'}$, $Y_{ee'cc'} = \tilde{D}_{ee'cc'}$, $Z_{ee'cc'} = D_{ee'cc'}$.

Three-body part.

\[
\Omega^{(2)+}_{\nu\nu'\nu''c'c''}(\Lambda_1\Lambda_2\Lambda_3)(\varepsilon_{\nu'c'} - \varepsilon_{\nu''v''})
\]

\[
= \frac{1}{2} \delta_{\Lambda_1\Lambda_3} \delta_{M,M_3} [\overline{T}_{\nu\nu''v''c'c'}(\Lambda_1\Lambda_2\Lambda) + \frac{1}{2} \overline{T}_{\nu\nu''v''c'c'}(\Lambda_1\Lambda_2\Lambda)] \\
- \sum_{\lambda_2\lambda_3} J_{\nu\nu''v''c'c'}(\Lambda_1\Lambda_2\Lambda_3\lambda) \{ \overline{T}_{\nu\nu''v''c'c'}(\Lambda_1\Lambda_2\Lambda) \} + (-1)^{\lambda_3 + \lambda_2} Y_{\nu\nu''v''c'c'}(\Lambda_1\Lambda_2\Lambda_3\tau_1) \\
\times T_{\nu\nu''v''c'c'}(\Lambda_1\tau_1) + \frac{1}{2} \sum_{\lambda} a(\lambda\nu'\nu u) \\
\times I_{\nu\nu''v''c'c'}(\Lambda_1\Lambda_2\Lambda_3\tau_1\tau_2)\tilde{T}_{\nu''v''c'c'}(u\tau_2),
\]

(A9a)

\[
\Omega^{(2)-}_{\nu\nu'\nu''c'c''}(\Lambda_1\Lambda_2\Lambda_3)(\varepsilon_{\nu'c'} - \varepsilon_{\nu''v''})
\]

\[
= \frac{1}{2} \delta_{\Lambda_1\Lambda_3} \delta_{M,M_3} a(\lambda\nu'\nu\lambda_1) [a(\lambda\nu'\nu\lambda_2) \overline{T}_{\nu\nu''c'c''}(\Lambda_2\Lambda_1\Lambda) \\
+ \sum_{\lambda_2\lambda_3} a(\lambda\nu'\nu\lambda_2) J_{\nu\nu''c'c'}(\Lambda_2\Lambda_2\Lambda_1) T_{c'c''\nu''v''}(\overline{\Lambda_2}\Lambda_1\Lambda)],
\]

(A9b)
\[ \Omega^{(2)+}_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{ee'c'} - \varepsilon_{vv'e'}) \]

\[ \begin{aligned} &= \delta_{\Lambda\Lambda_3}\delta_{MM_3}\{ -a(\lambda_c\lambda_{c'}\Lambda_2)T_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda) \\
&+ \frac{1}{2}\tilde{T}_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda) \} - a(\lambda_c\lambda_{v'}\Lambda_1)\{ T_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda) \\
&+ \frac{1}{2}\tilde{T}_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda) \} - \sum_{\nu} J_{vv'ee'c'}(\Lambda_2\Lambda_2\Lambda_2\Lambda_1) \\
&\times \{ \frac{1}{2}\tilde{T}_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda) \} + \tilde{T}_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda) \} + (-1)^{\lambda_c + \lambda_{v'}}Y_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda_3\tau_1) \\
&\times \tilde{T}_{vv'ee'c'}(\Lambda_1\tau_1) + \frac{1}{2}a(\lambda_c\lambda_{v}\Lambda_2)Y'_{vv'ee'}(\tau_1\Lambda_1\Lambda_3\Lambda_2) \\
&\times T_{vv'ee'c'}(\Lambda_2\tau_1) + \sum_{\nu} a(\lambda_c\lambda_{v'}\Lambda_2) \\
&\times I_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda_3\tau_1\Lambda u)T_{vv'ee'c'}(u\tau_1) + \frac{1}{2}a(\lambda_{v'}\lambda_{v}u) \\
&\times I_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\tilde{T}_{vv'ee'c'}(u\tau_2) + (-1)^{\lambda_c - \lambda_{v'}} \\
&\times a(\lambda_c\lambda_{v'}\Lambda_1)I_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda_3\tau_2\Lambda u)\tilde{T}_{vv'ee'c'}(u\tau_2) \} , \end{aligned} \]

\( (A10a) \)

\[ \Omega^{(2)-}_{vv'ee'c'}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{ee'c'} - \varepsilon_{vv'e'}) \]

\[ \begin{aligned} &= \delta_{\Lambda\Lambda_3}\delta_{MM_3}a(\lambda_c\lambda_{v'}\Lambda_1)[a(\lambda_c\lambda_{c'}\Lambda_2)\tilde{T}_{ee'c'}(\Lambda_2\Lambda_1\Lambda) \\
&+ \frac{1}{2}\sum_{\nu}\pi J_{ee'c'}(\Lambda_1\Lambda_2\Lambda_2\Lambda_1)\tilde{T}_{ee'c'}(\Lambda_2\Lambda_1\Lambda) \\
&\cdot (-1)^{\lambda_c - \lambda_{v}}\sum_{\nu} I'_{ee'c'}(\Lambda_1\Lambda_2\Lambda_1\Lambda\Lambda)T_{ee'c'}(\Lambda_1\Lambda_2\Lambda_1\Lambda) \\
&- a(\lambda_c\lambda_{v}\Lambda_2)\tilde{T}_{ee'c'}(\Lambda_2\Lambda_1\Lambda) \} ] . \end{aligned} \]

\( (A10b) \)
\[ \Omega^{(2)+}_{ee'vv'c'}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda)(\varepsilon_{vc'} - \varepsilon_{ee'}) = \delta_{\Lambda \Lambda_3} \delta_{MM_3} \left[ \frac{1}{2} \tilde{T}_{ee'vv'c'}(\tilde{\Lambda}_1 \Lambda_2 \Lambda) + \frac{1}{2} \tilde{T}_{ee'vv'c'}(\Lambda_1 \Lambda_2 \Lambda) \right] + a(\lambda_v \lambda_v' \Lambda_1) \{ a(\lambda_c \lambda_c' \Lambda_2) \tilde{T}_{ee'vv'c'}(\tilde{\Lambda}_1 \Lambda_2 \Lambda) \\
- \frac{1}{2} \tilde{T}_{ee'vv'c'}(\Lambda_1 \Lambda_2 \Lambda) \} + \sum_{\pi_2 \pi} J_{ecvc}(\overline{\Lambda}_2 \Lambda \Lambda_1) \\
\times \left\{ \frac{1}{4} (a(\lambda_c \lambda_v \Lambda_2) \tilde{T}_{ee'vv'c'v}(\Lambda_1 \overline{\Lambda}_2 \Lambda) \right. \\
- \left. \tilde{T}_{ee'vv'c'v}(\Lambda_1 \overline{\Lambda}_2 \Lambda) \right\} + a(\lambda_v \lambda_v' \Lambda_1) (\tilde{T}_{ee'vv'c'}(\Lambda_1 \overline{\Lambda}_2 \Lambda) + \tilde{T}_{ee'vv'c'}(\Lambda_1 \overline{\Lambda}_2 \Lambda)) \right\} \\
+ \delta_{\Lambda_1 \Lambda_2} \delta_{\Lambda_3 \tau_2} \delta_{\Lambda 0} T_{ee'vv'c'}(\Lambda_1 \tau_1) + (-1)^{\lambda_v + \lambda_v'} \\
\times Y_{ecvc}(\Lambda_1 \Lambda_2 \Lambda \Lambda_3 \tau_1) \tilde{T}_{ee'vv'c'v}(\Lambda_1 \tau_1) + \sum_{u} [a(\lambda_v \lambda_v' \Lambda_2) \\
\times I_{ee'vv'c'}(\Lambda_1 \Lambda_2 \Lambda_3 \tau_1 \Lambda u) T_{ee'vv'c'v}(u \tau_1) + a(\lambda_v \lambda_v' \Lambda_2) \\
\times \left\{ \frac{1}{2} I_{ee'vv'c'}(\Lambda_1 \Lambda_2 \Lambda_3 \tau_2 \Lambda u) \tilde{T}_{ee'vv'c'v}(u \tau_2) \\
+ (-1)^{\lambda_v - \lambda_v'} I_{ee'vv'c'}(\Lambda_1 \Lambda_2 \Lambda_3 \tau_2 \Lambda u) \tilde{T}_{ee'vv'c'v}(u \tau_2) \right\} \right], \]

\[ \Omega^{(2)-}_{ee'vv'c'}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda)(\varepsilon_{vc'} - \varepsilon_{ee'}) = \delta_{\Lambda \Lambda_3} \delta_{MM_3} a(\lambda_v \lambda_v' \Lambda_1) [a(\lambda_c \lambda_c' \Lambda_2) \tilde{T}_{ee'vv'c'}(\Lambda_2 \Lambda_1 \Lambda) \\
+ \frac{1}{2} \sum_{\pi_2 \pi} J_{ecvc}(\overline{\Lambda}_2 \Lambda \Lambda_1) \tilde{T}_{ee'vv'c'}(\Lambda_2 \Lambda_1 \overline{\Lambda}) \\
+ (-1)^{\lambda_v - \lambda_v'} \sum_{\tau_1} I_{ee'vv'c'}(\overline{\Lambda}_1 \overline{\Lambda}_2 \Lambda \Lambda_2 \Lambda) (T_{ee'vv'c'v}(\Lambda_2 \overline{\Lambda}_1 \overline{\Lambda}) \\
- a(\lambda_c \lambda_v \Lambda_2) \tilde{T}_{ee'vv'c'}(\Lambda_2 \overline{\Lambda}_1 \overline{\Lambda})) \right], \]

\[ \Omega^{(2)+}_{vv'vv'c'c'}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{vv'} - \varepsilon_{vv'}) = \frac{1}{2} \delta_{\Lambda \Lambda_3} \delta_{MM_3} \left[ \tilde{T}_{vv'vv'c'c'}(\Lambda_1 \Lambda_2 \Lambda) + \tilde{T}_{vv'vv'c'c'}(\Lambda_1 \Lambda_2 \Lambda) \right] + a(\lambda_v \lambda_v' \Lambda_2) \sum_{\pi_2 \pi} J_{vv'vc}(\overline{\Lambda}_2 \Lambda \Lambda_1) \tilde{T}_{vv'vv'c'c'}(\Lambda_1 \overline{\Lambda}_2 \Lambda) \right], \]

\[ \Omega^{(2)-}_{vv'vv'c'c'}(\Lambda_1 \Lambda_2 \Lambda)(\varepsilon_{vv'} - \varepsilon_{vv'}) = \delta_{\Lambda \Lambda_3} \delta_{MM_3} a(\lambda_v \lambda_v' \Lambda_2) \left[ \frac{1}{2} a(\lambda_c \lambda_v' \Lambda_1) \tilde{T}_{vv'vv'c'c'}(\Lambda_2 \Lambda_1 \Lambda) \\
- T_{vv'vv'c'c'}(\overline{\Lambda}_2 \Lambda_1 \Lambda) \right] \right]. \]
\[ \Omega_{vv'ev'c}^{(2)}(\Lambda_1\Lambda_2\Lambda_3\Lambda)(\varepsilon_{vv'c} - \varepsilon_{vv'}) \]

\[ = \delta_{\Lambda_1\Lambda_3} \delta_{MM_1} \frac{1}{2} \left\{ \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) + \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \right\} - a(\lambda_0\lambda_v\Lambda_1) \{ \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) + \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \} + a(\lambda_c\lambda_v\Lambda_2) \sum_{\pi_2=\pi} J_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \times \{ \frac{1}{2} \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) - \frac{1}{2} a(\lambda_0\lambda_v\Lambda_1) \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \} \]

\[ = \delta_{\Lambda_1\Lambda_3} \delta_{MM_1} \left[ \frac{1}{2} \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) - \frac{1}{2} a(\lambda_c\lambda_v\Lambda_2) \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \right] \]

\[ - a(\lambda_0\lambda_v\Lambda_1) \{ \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) + \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \} + a(\lambda_c\lambda_v\Lambda_2) \sum_{\pi_2=\pi} J_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda_1) \times \{ \frac{1}{2} \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) - \frac{1}{2} a(\lambda_0\lambda_v\Lambda_1) \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \} \times \{ \frac{1}{2} \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) - \frac{1}{2} a(\lambda_c\lambda_v\Lambda_2) \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \} \]

\[ \times \{ \frac{1}{2} \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) - \frac{1}{2} a(\lambda_0\lambda_v\Lambda_1) \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \} \times \{ \frac{1}{2} \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) - \frac{1}{2} a(\lambda_c\lambda_v\Lambda_2) \tilde{T}_{vv'ev'c}(\Lambda_1\Lambda_2\Lambda) \} \]
\[
\Omega_{ee'vv'\nu c}^{(2)+}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda)(\varepsilon_{vv'c} - \varepsilon_{ee'v})
\]

\[
= \delta_{\Lambda \Lambda_3} \delta_{MM_3} \left[ \frac{1}{2} \left\{ \tilde{T}_{ee'vv'c}(\Lambda_1 \Lambda_2 \Lambda) + \tilde{T}_{ee'vv'c}(\Lambda_1 \Lambda_2 \Lambda) \right\} 
- a(\lambda_{e'} \lambda_{e} \Lambda_1) \{ \tilde{T}_{ee'vv'c}(\Lambda_1 \Lambda_2 \Lambda) + \tilde{T}_{ee'vv'c}(\Lambda_1 \Lambda_2 \Lambda) \} 
+ a(\lambda_e, \lambda_{e'} \Lambda_2) \sum_{\overline{\Lambda}_2} \frac{1}{2} \tilde{T}_{ee'vv'v'}(\overline{\Lambda}_1 \overline{\Lambda}_2 \overline{\Lambda}) 
- a(\lambda_{e'} \lambda_{e} \Lambda_1) \left( \frac{1}{2} \tilde{T}_{ee'vv'v'}(\Lambda_1 \overline{\Lambda}_2 \overline{\Lambda}) + \tilde{T}_{ee'vv'v'}(\Lambda_1 \overline{\Lambda}_2 \overline{\Lambda}) \right) \right] 
+ \delta_{\Lambda_1 \Lambda_2} \delta_{\Lambda_1 \Lambda_1} a(\lambda_e \lambda_{e'} \Lambda_1) \left( -1 \right)^{\Lambda_2} 
\times Y_{ee'vv'c}(\Lambda_1 \Lambda_2 \Lambda_3 \tau_1) T_{ee'vv'v'}(\Lambda_1 \tau_1) 
+ \frac{1}{2} a(\lambda_{e'} \lambda_{e} \Lambda_1) 
\times \{ I_{ee'vv'c}(\Lambda_1 \Lambda_2 \Lambda_3 \tau_1 \Lambda u) T_{ee'vv'v'}(\Lambda_1 \tau_1) \}
\] (A14a)

\[
\Omega_{ee'vv'\nu c}^{(2)-}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda)(\varepsilon_{vv'c} - \varepsilon_{ee'v})
\]

\[
= -\delta_{\Lambda \Lambda_3} \delta_{MM_3} \left[ a(\lambda_{e} \lambda_{e'} \Lambda_1) \{ \tilde{T}_{ee'vv'v'}(\Lambda_2 \Lambda_1 \Lambda) \}
- \frac{1}{2} a(\lambda_{e} \lambda_{e'} \Lambda_2) \tilde{T}_{ee'vv'v'}(\Lambda_2 \Lambda_1 \Lambda) \right] (A14b)
+ \frac{1}{2} a(\lambda_{e} \lambda_{e'} \Lambda_2) \sum_{\overline{\Lambda}_2} a(\lambda_{e} \lambda_{e'} \overline{\Lambda}_1) a(\lambda_{e} \lambda_{e'} \overline{\Lambda}_2) \left( -1 \right)^{\Lambda_2} 
\times \tilde{T}_{ee'vv'v'}(\overline{\Lambda}_1 \overline{\Lambda}_2 \Lambda_1 \Lambda \overline{\Lambda}) T_{ee'vv'v'}(\overline{\Lambda}_2 \Lambda_1 \Lambda \overline{\Lambda}) 
+ \frac{1}{2} \tilde{T}_{ee'vv'v'}(\overline{\Lambda}_1 \overline{\Lambda}_2 \Lambda_1 \Lambda \overline{\Lambda}) \tilde{T}_{ee'vv'v'}(\overline{\Lambda}_2 \Lambda_1 \Lambda \overline{\Lambda}) \right].
\]

**Four-body part.**

\[
\Omega_{vv'vv'\nu'\nu c}^{(2)}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda_4 \Lambda)(\varepsilon_{vv'c} - \varepsilon_{vv'\nu'\nu'})
\]

\[
= \frac{1}{2} ( -1 )^{\Lambda_3} a(\lambda_{e} \lambda_{e'} \Lambda_1) F_{c'vv'}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda_4 \Lambda) 
\times Q_{vv'vv'\nu'\nu c'}(\Lambda_1 \Lambda_3).
\] (A15)
\[\Omega^{(2)}_{\epsilon\epsilon'\nu'\nu'\epsilon'\epsilon'}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda_4 \Lambda)(\epsilon\epsilon'\epsilon') - \epsilon\epsilon'\epsilon'\nu')\]

\[= \frac{i}{4} \delta_{\Lambda_1 \Lambda_2} \delta_{\Lambda_3 \Lambda_4} \delta_{\Lambda_0} \{Q_{\epsilon\epsilon'\nu'\nu'\epsilon'\nu'}(\bar{\Lambda}_1 \Lambda_3) + Q_{\nu'\nu'\epsilon'\epsilon'\nu'\nu'}(\bar{\Lambda}_3 \Lambda_1)\} - \frac{i}{4} (-1)^{A_3} \{F_{\epsilon'\epsilon'}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda_4 \Lambda)Q_{\epsilon\epsilon'\nu'\nu'\epsilon'\nu'}(\bar{\Lambda}_1 \Lambda_3) + (-1)^{A_3} a(\lambda_e \lambda_4 \Lambda_1)\]

\[+ (-1)^{A_1+4} F_{\epsilon'\epsilon'}(\Lambda_4 \Lambda_3 \Lambda_2 \Lambda_1 \Lambda)Q_{\epsilon\epsilon'\nu'\nu'\epsilon'\nu'}(\bar{\Lambda}_4 \Lambda_2)\]

\[+ a(\lambda_e \lambda_4 \Lambda_1) a(\lambda_4 \lambda_2 \Lambda_1) F_{\epsilon'\epsilon'}(\Lambda_1 \Lambda_2 \Lambda_3 \Lambda_4 \Lambda)\]

\[\times Q_{\epsilon'\epsilon'\epsilon'\epsilon'\epsilon'}(\bar{\Lambda}_3 \Lambda_1) + a(\lambda_4 \lambda_2 \Lambda_1) a(\lambda_4 \lambda_2 \Lambda_1)\]

\[\times F_{\epsilon'\epsilon'}(\Lambda_4 \Lambda_3 \Lambda_2 \Lambda_1 \Lambda)Q_{\epsilon\epsilon'\nu'\nu'\epsilon'\nu'}(\bar{\Lambda}_4 \Lambda_2)\]

\[+ \sum_{ud} G_{\epsilon'\epsilon'\nu'\nu'\epsilon'\nu'}(ud \Lambda_1 \Lambda_3 \Lambda_2 \Lambda_4 \Lambda)\]

\[\times G_{\epsilon'\epsilon'\epsilon'\epsilon'\epsilon'}(ud \Lambda_1 \Lambda_3 \Lambda_2 \Lambda_4 \Lambda).\]

The coefficients \(J, Y, Y', I, I', F, G\) are defined by the following formulas

\[J_{\alpha \beta \bar{\rho}}(\Lambda_1 \Lambda_2 \bar{\Lambda}_1 \bar{\Lambda}_2 \Lambda) = (-1)^{\Lambda_2+\bar{\Lambda}_2} [A_1][\Lambda_2, \bar{\Lambda}_2, \bar{\Lambda}_2]^{1/2} \left\{ \begin{array}{c} \lambda_\alpha \\ \lambda_\beta \\ \lambda_\rho \\ \bar{\Lambda}_1 \\ \bar{\Lambda}_2 \\ \Lambda \end{array} \right\}, \quad (A18)\]

\[Y_{\alpha \beta \bar{\rho}}(\Lambda_1 \Lambda_2 \bar{\Lambda}_1 \bar{\Lambda}_2 \Lambda) = (-1)^{\Lambda_1+\bar{\Lambda}_1+\bar{\Lambda}_2} [A_1, \Lambda_2, \Lambda_1]^{1/2} \times \left\{ \begin{array}{c} \lambda_\alpha \\ \lambda_\beta \\ \lambda_\rho \\ \bar{\Lambda}_1 \\ \bar{\Lambda}_2 \\ \Lambda \end{array} \right\}, \quad (A19)\]

\[Y'_{\alpha \beta \bar{\rho}}(\Lambda_1 \Lambda_2 \bar{\Lambda}_1 \bar{\Lambda}_2 \Lambda) = (-1)^{\Lambda_1+\Lambda_2} [A_1, \Lambda_1, \Lambda_2]^{1/2} \times \left\{ \begin{array}{c} \bar{\Lambda}_1 \\ \Lambda_2 \Lambda_1 \Lambda_2 \Lambda \end{array} \right\}; \quad (A20)\]

\[I_{\alpha \beta \bar{\rho} \theta}(\Lambda_1 \Lambda_2 \bar{\Lambda}_1 \bar{\Lambda}_2 \Lambda \bar{\Lambda}) = (-1)^{\Lambda_1+\bar{\Lambda}_1} [\Lambda_1, \bar{\Lambda}_2, \Lambda, \bar{\Lambda}]^{1/2} \times \left\{ \begin{array}{c} \bar{\Lambda}_1 \\ \Lambda_2 \Lambda_1 \Lambda_2 \Lambda \end{array} \right\}, \quad (A21)\]
REFERENCES

A. Derevianko, J. Phys. B: At. Mol. Opt. Phys. 43, 074001 (2010).
Vilnius, 1984).

28 H. Sh. Chou, Phys. Rev. A 62, 042507 (2000).