Symbolic programming package \textit{NCoperators} with applications to theoretical atomic spectroscopy

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Abstract. A symbolic programming package \textit{NCoperators} with applications to atomic physics is introduced. The package runs over \textit{Mathematica} and it implements \textit{NCAlgebra}, the noncommutative algebra package. \textit{NCoperators} features the algebra of irreducible tensor operators, the second quantization representation, the angular momentum theory, and the effective operator approach exploited in many-body perturbation theory, including Wick’s theorem. The comprehensiveness is yet another characteristic feature of the present package: The generation of expressions is performed in a way as if it were done by hand. Although the theoretical atomic spectroscopy is a direct target of \textit{NCoperators}, the package, with minor modifications, if any, is believed to appropriate other areas of theoretical physics as well.

1. Introduction
To this day, a number of \textit{Mathematica} sources featuring the properties of creation and annihilation operator products are observed in literature: \textit{Nostromo} [1], \textit{SeQuant} [2], \textit{Wick} [3], \textit{Quantum} [4], \textit{SNEG} [5] etc. Against the variety of areas of theoretical physics the packages supply with, none of them provide an opportunity to manage the Racah algebra [6–8] in a fully compatible fashion; the capability of constructing the irreducible tensor form of complex operators that act on the basis of many-electron open-shell wave functions is advantageous in a special manner. The package \textit{NCoperators} is just what one needs to solve this kind of tasks [9] along with many other ones, eg. the summation of Clebsch–Gordan products to the $3nj$–symbols [10]. Whilst the \textit{Racah} package [11–13], based on \textit{Maple}, is known to handle several similar procedures such as the calculation of transformation matrices and recoupling coefficients, evaluation of many-particle matrix elements etc., the advantages and distinctive features of \textit{NCoperators} are that (i) it manages the reduction of the product of more than two SU(2)–irreducible representations therefore giving an opportunity to calculate the matrix elements on the basis of many-open-shell wave functions (eg. six open shells appear even in the second-order Rayleigh–Schrödinger perturbation theory based on effective operator approach [14]); (ii) it is based on the algebraic manipulations of the quantities considered neither the diagrammatic representations such as the Jucys graphs exploited in the angular momentum theory [15], though the diagrammatic visualization, to some extent, is implemented as well; (iii) the output of expressions, including Clebsch–Gordan coefficients and $3nj$–symbols, obtained within \textit{Mathematica} interface fits the standard text-based form; (iv) \textit{Racah} refers to Varshalovich et al [16], while \textit{NCoperators} implements the sum rules given by Jucys et al [15; 17]; in many
particular cases, the difference is in the phase factor and different notions (e.g., the Clebsch–
Gordan coefficient versus the Wigner \(3j\)-symbol): (v) at last, but not least, the package \(NC\) _operators_ allows one to generate expansion terms of the Rayleigh–Schrödinger perturbation theory up to the third-order \([18]\), and afterward express them in the irreducible tensor form. To calculate energy corrections, such an operator representation puts into direct action the technique that was first proposed by Judd \([19]\) and later extensively developed by Rudzikas et al. \([20–22]\).

At the present moment, the package under consideration is used for private research purposes only, though the source files can be sent directly to anyone concerned with the subject.

In this paper, we review the package \(NC\) _operators_ from the perspectives of what it is likely for the application of techniques exploited in modern theoretical atomic spectroscopy.

### 2. Effective operator approach in RSPT

Our proposed formulation of the Rayleigh–Schrödinger perturbation theory (RSPT) relies on the following statement \([9, \text{Theorem 2.7}]\): The nonzero terms of effective Hamiltonian, \(\mathcal{H}^*\), on the model space \(\mathcal{P}\) are generated by a maximum of eight types of the \(n\)-body parts of wave operator, \(\Omega\), with respect to the single-electron states of the set \(I_n(\alpha\beta)\) for all \(n \geq 1\).

Several results immediately proceed from the present statement. First, it allows us to reduce significantly the number of \(n\)-body parts of \(\Omega\), denoted \(\Omega_n\), that are generated by using the generalized Bloch equation \([18]\). That is to say, only 8 of the \(9^n\) possible distributions of single-electron states (valence, core, excited) have non-zero contribution to the expansion series of \(\mathcal{H}^*\). Second, both approaches the coupled-cluster (CC) and the RSPT are treated similarly by means of the tensor form of expansion terms – it is only the scalar multiplier (also known as the effective matrix element calculated on the basis of single-particle wave functions) that separates CC and RSPT. Therefore, once the irreducible tensor form of \(\mathcal{H}^*\) is constructed, one can easily make the replacements of routine multipliers depending on whether CC or RSPT approach is imposed on. In particular, the package \(NC\) _operators_ generates the terms in the RSPT approximation.

Let us clarify the above proposed statement in a more detail. Let \(\alpha\) and \(\beta\) denote the single-electron states the creation operator \(a_\alpha\) creates and the annihilation operator \(a_\beta^\dagger\) annihilates.

The single-electron states are valence (v), core (c) and excited or virtual (e). Then the model space \(\mathcal{P}\) is constructed by declaring that (A) \(a_\alpha \hat{P} = 0\), (B) \(a_\beta^\dagger \hat{P} = 0\), (C) \(a_\nu \hat{P} \neq 0\), and (D) \(a_\nu^\dagger \hat{P} \neq 0\). Here, \(\hat{P}\) denotes the projection operator that projects vectors in \(\mathcal{H}\), the \(N\)-electron Hilbert space, onto the vectors in \(\mathcal{P}\); one assumes that the initially given Hamiltonian \(\hat{H}\) acts on \(\mathcal{H}\), whereas the effective Hamiltonian \(\mathcal{H}^*\) acts on \(\mathcal{P}\). That is, the effective Hamiltonian reads

\[
\mathcal{H}^* = \hat{P} \hat{H} \hat{P} + \sum_{n=1}^{\infty} \sum_{m=1}^2 \sum_{\xi=1}^{\min(2m,2n)} \{\hat{P} \hat{V}_m \hat{\Omega}_n \hat{P}\}_{\xi},
\]

which is obtained by applying the Wick’s theorem (: denotes the normal ordering, \(\xi\) denotes the \(\xi\)-pair contraction between \(\hat{V}_m\) and \(\hat{\Omega}_n\)). The quantities \(\hat{V}_1\) and \(\hat{V}_2\) denote the single-particle and two-particle interaction operators. The wave operator \(\hat{\Omega}_n\) is of the form

\[
\hat{\Omega}_n = \sum_{I_n(\alpha\beta)} :Q_a\alpha_1 a_\alpha_2 \ldots a_\alpha_{n-1} a_\alpha_n a_\beta_1 a_\beta_2 \ldots a_\beta_{n-1} a_\beta_n :\hat{P} :\omega_n(\alpha\beta),
\]

for \(Q\) is the orthogonal complement of \(\hat{P}\). Here, \(\omega_n(\alpha\beta)\) is the above mentioned effective \(n\)-particle matrix element with the energy denominator included. The set \(I_n(\alpha\beta) = \{\alpha_1, \alpha_2, \ldots, \alpha_{n-1}, \alpha_n, \beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n\}\). In agreement with items (A)-(D), \(\hat{\Omega}_n\) is nonzero if and only if the \(\alpha_i\) states are valence and/or excited, while the \(\beta_j\) states are valence and/or core. In addition, \(\hat{\Omega}_n\)
is zero if and only if the sum of SO(3)-irreducible representations \( l_{\nu_i} + l_{\psi_i} \) over all \( i = 1, 2, \ldots, n \) is even,

\[
\sum_{i=1}^{n} (l_{\nu_i} + l_{\psi_i}) \equiv 0 \mod 2. \tag{3}
\]

Eq. (3) may be thought of as an additional parity selection rule that directly follows from items (C)-(D). A subsequent result is the initially proposed statement. In agreement with the parity selection rule, the wave operator \( \hat{\Omega}_n \), eq. (2), that distinguishes between single-, two-, three-, four-particle effects \((n = 1, 2, 3, 4)\) reads

\[
\hat{\Omega}_1 = \sum_{I_1^{(1)}} a_{\nu} a_{\psi}^\dagger \bar{\omega} \varepsilon + \sum_{I_1^{(2)}} a_{\nu} a_{\psi}^\dagger \bar{\omega} \varepsilon + \sum_{I_1^{(3)}} a_{\nu} a_{\psi}^\dagger \bar{\omega} \varepsilon, \tag{4a}
\]

\[
\hat{\Omega}_2 = \sum' a_{\nu} a_{\nu'}^\dagger a_{\psi}^\dagger a_{\psi'}^\dagger \bar{\omega} \alpha \alpha' \beta \beta' + \sum_{I_2^{(3)}} a_{\nu} a_{\nu'}^\dagger a_{\psi}^\dagger \bar{\omega} \varepsilon \varepsilon \varepsilon \varepsilon + \sum' a_{\nu} a_{\nu'}^\dagger a_{\psi}^\dagger \bar{\omega} \varepsilon \varepsilon \varepsilon \varepsilon + \sum' a_{\nu} a_{\psi}^\dagger a_{\psi'}^\dagger \bar{\omega} \varepsilon \varepsilon \varepsilon \varepsilon, \tag{4b}
\]

\[
\hat{\Omega}_3 = \sum' a_{\nu} a_{\nu'}^\dagger a_{\nu''}^\dagger a_{\psi}^\dagger a_{\psi'}^\dagger a_{\psi''}^\dagger \bar{\omega} \alpha \alpha' \beta \beta' \beta'' \beta''' \beta'''' \beta''''' + \sum' a_{\nu} a_{\nu'}^\dagger a_{\alpha}^\dagger a_{\beta}^\dagger a_{\beta'}^\dagger \bar{\omega} \varepsilon \varepsilon \varepsilon \varepsilon \varepsilon \varepsilon \varepsilon \varepsilon \varepsilon \varepsilon, \tag{4c}
\]

\[
\hat{\Omega}_4 = \sum' a_{\nu} a_{\nu'}^\dagger a_{\alpha}^\dagger a_{\beta}^\dagger a_{\beta'}^\dagger a_{\beta''}^\dagger \bar{\omega} \alpha \alpha' \alpha'' \beta \beta' \beta'' \beta''' \beta'''' \beta''''' \beta'''''. \tag{4d}
\]

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:

\[
\sum' \equiv \sum_{I_2^{(4,5,8)}} \delta_{\alpha \alpha'} \delta_{\beta \beta'} + \sum_{I_2^{(6)}} \delta_{\alpha \beta} \delta_{\beta \alpha' \beta'} + \sum_{I_2^{(8)}} \delta_{\alpha \beta} \delta_{\beta \beta'}, \tag{5a}
\]

\[
\sum' \equiv \sum_{I_2^{(4,5,8)}} \delta_{\beta \beta'} + \sum_{I_2^{(6)}} \delta_{\beta \beta'} \text{ for } x = 2, a = 1, b = 6 \text{ and } x = 3, 4, a = 2, b = 5, \tag{5b}
\]

\[
\sum' \equiv \sum_{I_2^{(4,5,8)}} \delta_{\beta \beta'} + \sum_{I_2^{(6)}} \delta_{\beta \beta'} \text{ for } x = 2, a = 2, b = 7 \text{ and } x = 4, a = 1, b = 4, \tag{5c}
\]

\[
\sum' \equiv \sum_{I_2^{(4,5,8)}} \delta_{\alpha \nu} \delta_{\mu \nu} + \sum_{I_2^{(6)}} \delta_{\alpha \nu} \delta_{\mu \nu}, \tag{5d}
\]

\[
\sum' \equiv \sum_{I_2^{(3)}} \delta_{\alpha \nu} \delta_{\beta \nu} + \sum_{I_2^{(6)}} \delta_{\alpha \nu} \delta_{\beta \nu} + \sum_{I_2^{(7)}} \delta_{\alpha \nu} \delta_{\beta \nu} + \sum_{I_2^{(8)}} \delta_{\alpha \nu} \delta_{\beta \nu}, \tag{5e}
\]
\[ \sum_{I_4(3,6,7,8)} \equiv \sum_{I_4(3)} \delta_{\alpha \nu} \delta_{\beta \nu} + \sum_{I_4(6)} \delta_{\alpha \nu} \delta_{\beta c} + \sum_{I_4(7)} \delta_{\alpha e} \delta_{\beta c} + \sum_{I_4(8)} \delta_{\alpha e} \delta_{\beta c}. \quad (5f) \]

As seen from eq. (5), no more than eight types of sets \( I_n(\alpha \bar{\beta}) \) are observed: Although each \( \hat{\Omega}_n \) contains more terms than those in eq. (4), but only the displayed eight types of sets \( I_n(\alpha \bar{\beta}) \) have nonzero contribution to the effective Hamiltonian \( \hat{H} \), eq. (1).

In particular, one may express the third-order effective Hamiltonian \( \hat{H}^{(3)} \) by

\[ \hat{H}^{(3)} = \sum_{I_{m+n-\xi}} \sum_{m=1}^{2} \sum_{n=1}^{4} \sum_{\xi=1}^{\min(2m,2n)} \xi \{ \hat{P} \hat{V}_1 \hat{\Omega}^{(2)}_1 \hat{P} \}_{\xi}. \quad (6) \]

where \( \hat{\Omega}^{(2)}_1 \) is given by eq. (4) with the effective matrix elements \( \omega_n(\alpha \bar{\beta}) \) replaced by the second-order effective matrix elements \( \omega_n^{(2)}(\alpha \bar{\beta}) \). \( I_{m+n-\xi} \) denotes the set of all single-particle orbitals.

Even if eq. (3) is exploited, there are hundreds of generated \( \hat{\Omega}^{(2)}_n \) and \( \hat{H}^{(3)} \) terms. Therefore, the role of \( NCoperators \) becomes essential.

3. The generation of expansion terms

The package \( NCoperators \) takes into consideration the anticommutation properties of creation and annihilation operators, \( \{ a_{\alpha i}, a^\dagger_{\beta j} \} = \delta(\alpha_i, \beta_j), \{ a_{\alpha i}, a_{\beta j} \} = 0, \{ a^\dagger_{\alpha i}, a^\dagger_{\beta j} \} = 0 \). The realization is illustrated in Fig. 1.

![Figure 1. Manipulating anticommutation properties of creation and annihilation operators in NCoperators. The outputs Out[59] and Out[62] are fully compatible with \LaTeX.](image)

As a representative example, let us consider the single-particle operator \( \{ \hat{P} \hat{V}_1 \hat{\Omega}^{(2)}_1 \hat{P} \}_1 \): The interaction operator \( \hat{V}_1 = \sum_{\alpha \bar{\beta}} a_{\alpha i} a^\dagger_{\beta j} v_{\alpha i} \), where \( v_{\alpha i} \) is the single-particle matrix element. By eq. (4a), the wave operator

\[ \hat{\Omega}^{(2)}_1 = \sum_{ev} a_e a^\dagger_{ev} \omega^{(2)}_{ev} + \sum_{vc} a_v a^\dagger_{vc} \omega^{(2)}_{vc} + \sum_{ec} a_e a^\dagger_{ec} \omega^{(2)}_{ec}. \quad (7) \]

The generation of \( \{ \hat{P} \hat{V}_1 \hat{\Omega}^{(2)}_1 \hat{P} \}_1 \) terms is performed in Fig. 2. In \( NCoperators \), the single-electron states are designated by
In a standard output (such as Out[4] in Fig. 2), the notation of orbitals is simplified to

\[ c : a_1, b_1, c_1, d_1, e_1, f_1 \]
\[ v : m_1, n_1, p_1, q_1, k_1, l_1 \]
\[ e : r_1, s_1, t_1, u_1, w_1, x_1 \]

One can recognize that the function \( \text{OneContraction}[2, \mu, \nu, 2, vc1, ca1] \) corresponds to the term at the sum \( \sum \) in eq. (7); similarly, the rest two functions \( \text{OneContraction}[2, \mu, \nu, 2, ec1, ca1] \) and \( \text{OneContraction}[2, \mu, \nu, 2, ec1, va1] \) correspond to the terms at \( \sum \) and \( \sum \), respectively. In Out[4], the effective matrix element \( \langle x | v^e_{\text{eff}} | y \rangle \) denotes \( \omega(2)_{xy}(\varepsilon_y - \varepsilon_x) \); \( \varepsilon_x \) is the single-electron energy, also observed in \( \hat{H}_0 = \sum_\alpha a_\alpha a_\alpha^\dagger \varepsilon_\alpha \). Other functions such as \( \text{KronDelta[]} \), \( \text{NormalOrder[]} \), \( \text{MatrixEl[]} \) should be obvious to identify by their names. Therefore, Out[4] shows us that the generated \( \{\hat{P}\hat{V}_1\hat{\Omega}^{(2)}\hat{P}\}_1 \): terms are

\[
\langle x | v^e_{\text{eff}} | y \rangle = \omega(2)_{xy}(\varepsilon_y - \varepsilon_x) - \sum_{cv} a_v a_c^\dagger v_{cv}\omega(2)_{cv} - \sum_{cv} a_v a_c^\dagger v_{cv}\omega(2)_{cv}.
\]

The next step is to obtain the scalars \( \omega(2)_{\alpha\beta} \). This is the most time consuming process. In agreement with the generalized Bloch equation, \( \omega(2)_{\alpha\beta} \) represents the sum of coefficients \( \omega(2)_{ij:j-1}(\alpha\beta) \) obtained from the terms \( \{\hat{R}\hat{V}_j\hat{\Omega}^{(1)}\hat{P} - \hat{R}\hat{\Omega}^{(1)}\hat{P}\hat{V}_j\hat{P}\}_{i+j-1} \); \( \hat{R} \) denotes the resolvent. Thus,

\[
\omega(2)_{\alpha\beta} = \omega(2)_{11}(\alpha\beta) + \omega(2)_{12}(\alpha\beta) + \omega(2)_{21}(\alpha\beta) + \omega(2)_{22}(\alpha\beta).
\]
In Figs. 3-4, the algorithms for obtaining the multipliers $\omega^{(2)}_{11,1}$ are displayed. As seen, $\omega^{(2)}_{11,1}$ consists of nine terms in total.

$$\omega^{(2)}_{11,1}(\vec{\alpha} \beta)(\vec{\varepsilon} - \varepsilon_\alpha) = \sum_{\mu} v_{\alpha \mu} \omega^{(1)}_{\mu \beta} - \sum_{\nu} v_{\nu \beta} \omega^{(1)}_{\nu \alpha},$$

where $\omega^{(1)}_{\alpha \beta} = v_{\alpha \beta}(\varepsilon_{\beta} - \varepsilon_\alpha)$ is the effective matrix element drawn in $\hat{\Omega}^{(1)}$. If performing analogous computations for the remaining coefficients $\omega^{(2)}_{ij,j-1}$, one finds that

$$\omega^{(2)}_{12,2}(\vec{\alpha} \beta)(\vec{\varepsilon} - \varepsilon_\alpha) = \sum_{c} \sum_{\mu,\nu,\epsilon} v_{\epsilon \mu} \left( \omega^{(1)}_{\mu \alpha \beta} - \omega^{(1)}_{\mu \beta \alpha} \right),$$

$$\omega^{(2)}_{21,2}(\vec{\alpha} \beta)(\vec{\varepsilon} - \varepsilon_\alpha) = \sum_{c} \sum_{\mu,\nu,\epsilon} \left( v_{\epsilon \mu \alpha \beta} - v_{\epsilon \mu \beta \alpha} \right) \omega^{(1)}_{\mu \epsilon},$$

$$\omega^{(2)}_{22,3}(\vec{\alpha} \beta)(\vec{\varepsilon} - \varepsilon_\alpha) = \sum_{c,\nu,\epsilon,\delta} \left( v_{\epsilon \mu \alpha \beta} - v_{\epsilon \nu \alpha \beta} \right) \left( \omega^{(1)}_{\epsilon \nu \beta \delta} - \omega^{(1)}_{\epsilon \nu \delta \beta} \right),$$

where $\omega^{(1)}_{\alpha \beta \rho} = v_{\alpha \beta \rho}(\varepsilon_{\beta} + \varepsilon_\rho - \varepsilon_\alpha - \varepsilon_\beta); v_{\alpha \beta \rho}$ denotes a two-particle matrix element. Finally, obtained coefficients $\omega^{(2)}_{\alpha \beta}$ are substituted in eq. (8). The same procedure should be carried out for the rest $\{\hat{P} \hat{V} \hat{\Omega}^{(1)} \hat{P}\}_{\xi}$: terms in order to establish all terms of $\hat{H}^{(3)}$ (see eq. (6)). The last step is to represent obtained expressions in the irreducible tensor form.

Figure 3. Generating the $\{\hat{R} \hat{V} \hat{\Omega}^{(1)} \hat{P}\}$: terms.
4. The irreducible tensor form of expansion terms

As first demonstrated by Judd [19], the operator $a_\alpha$ represents the irreducible tensor operator of SU$_J$(2) (in $jj$–representation) or SO$_L$(3) × SU$_S$(2) (in $LS$–representation). This operator is denoted by $a_\lambda^\alpha$, where $\lambda \equiv j$ or $\lambda \equiv \frac{1}{2}$. Note that in the $LS$–representation, $a_\lambda^\alpha$ represents a double tensor. According to this, we introduce a general form

$$\{\hat{P}\hat{V}_m\hat{\Omega}^{(2)}\}_{\xi} = \sum_{\Lambda} \sum_{\Gamma} \hat{O}_\Lambda^\Gamma([w]\varkappa) C^{(3)}_{mnm\xi}(\Gamma\Lambda),$$

for $\hat{O}_\Lambda^\Gamma([w]\varkappa)$ is the irreducible tensor operator of rank $\Lambda$; this notation fits both representations. The coefficient $C^{(3)}_{mnm\xi}(\Gamma\Lambda)$ is SU(2)–invariant. The letter $\Gamma$ denotes additional numbers necessary to obtain the above expression. The letter $w$ labels irreducible representations of $S_{2(m+n-\xi)}$, the symmetric group; these are of the type $[w] = [2^k1^h]$. $\varkappa$ denotes additional numbers, if necessary, in order to distinguish different reduction schemes of $\hat{O}_\Lambda^\Gamma([w]\varkappa)$. As one can easily observe, the $S_{2(m+n-\xi)}$–irreducible representations $[w]$ label the irreducible tensor operators $\hat{O}_\Lambda^\Gamma([w]\varkappa)$ associated with the $(m+n-\xi)$–particle operators $\{\hat{P}\hat{V}_m\hat{\Omega}^{(2)}\}_{\xi}$. For example, $\hat{O}_\Lambda^\Gamma([1^2]) = [a_\lambda^\alpha \times \tilde{a}_\lambda^\alpha]^\Lambda$, where $\tilde{a}_\lambda^\alpha$ denotes the irreducible tensor operator obtained from the transposed annihilation operator. The complete classification of irreducible tensor operators obtained by reducing the products of creation and annihilation operators one can find in [10].

The matrix elements of irreducible tensor operators of rank $\Lambda$ calculated on the basis of many-electron wave functions can be found, for example, in [20; 22]. For this reason, the SU(2)–invariants $C^{(3)}_{mnm\xi}(\Gamma\Lambda)$ are to be established to complete the task. As it appears from eq. (9), that the structure of $C^{(3)}_{mnm\xi}(\Gamma\Lambda)$ depends on $([w]\varkappa)$, that is to say, the reduction scheme. In turn, the
number of possible schemes depends on $m + n - \xi$. Obviously, for a fixed $m + n - \xi$, all reduction schemes are equivalent, and they are related by recoupling coefficients. These coefficients can be found by exploiting NCoperators.

Figure 5. The computation of recoupling coefficient with NCoperators. The phase factor can be reduced by applying the triangle rule.

For example, the computation of recoupling coefficient
is illustrated in Fig. 5. The quantity \( \left\{ \frac{j_1}{m_1}, \frac{j_2}{m_2}, \frac{j}{m} \right\} \) denotes the Clebsch–Gordan coefficient for the tensor product \( j_1 \times j_2 \rightarrow j \). \( \{ a \ b \ c \ d \ e \ f \} \) is the 6j-symbol. In Fig. 5, the obtained coefficient must be multiplied by \( (-1)^{2(a_4+a_5)+a_6+a_5+a_6(2\alpha_4+1)(2\alpha_5+1)} \) due to the recoupling in \( \left[ \begin{array}{ccc} a_4 & a_5 & a_5 + a_6 \\ a_4 & a_5 & a_5 + a_6 \\ a_4 & a_5 & a_5 + a_6 \end{array} \right] \).

Let us give a brief examination of the example studied above, in eq. (8). For the irreducible tensor operator a reduction scheme is labeled by the \( S_2 \)–irreducible representation \([1,2]\), the associated coefficient \( C_{11:1}^{(3)} \) is found by pulling out the \( SU(2) \)–invariant parts from the following products of matrix elements (see eq. (8)): \( \sum_{m_0} \omega_{e \bar{v} v_c}^{(2)} \) and \( \sum_{m_0} \omega_{e \bar{v} v_c}^{(2)} \), where the superscript \( \pm \) indicates the sign of \( \Lambda \) in eq. (9). The final result for the plus sign is,

\[
C_{11:1}^{(3)}(m_0 \Lambda) = (-1)^{\Lambda} \sqrt{2\tau_0 + 1} \sum_{x} \sqrt{2\tau_1 + 1} \left[ \begin{array}{ccc} \tau_0 & x & \Lambda \\ m_0 & M - m_0 & M \end{array} \right] \\
\times \left( (-1)^{A} \sum_{e} f(\tau_0 \lambda_v \lambda_e) \Omega_{v_e}^{(2)}(x) \left[ \begin{array}{ccc} \tau_0 & x & \Lambda \\ \lambda_v & \lambda_e & \lambda_e \end{array} \right] \right) \\
- (-1)^{x} \sum_{c} f(\tau_0 \lambda_v \lambda_c) \Omega_{v_c}^{(2)}(x) \left[ \begin{array}{ccc} \tau_0 & x & \Lambda \\ \lambda_v & \lambda_e & \lambda_e \end{array} \right],
\]

where \( f(\tau_1 \lambda_\alpha \lambda_\beta) = -\{(2\lambda_\alpha + 1)/(2\lambda_\beta + 1)\}^{1/2} \left[ n_\alpha \lambda_\alpha \|| v_\tau \|| n_\beta \lambda_\beta \right] \) is proportional to the reduced matrix element of interaction operator \( v_\tau \), \( i = 0, 1, 2 \). This matrix element is calculated on the basis of spherical harmonics. In particular, \( i = 0 \) befits the interaction drawn in the second quantized form of \( \hat{V}_1 \) in \( \{ \hat{P} \hat{V}_1 \hat{P} \}_1 \). The coefficients \( \Omega_{(a \beta)}^{(2)}(x) \) are found from

\[
\omega_{(a \beta)}^{(2)} = (-1)^{\lambda_\alpha + m_\beta} \sum_{x} \left[ \begin{array}{ccc} \lambda_\alpha & -m_\beta & \Lambda \\ m_\alpha & \lambda_\beta & M \end{array} \right] \Omega_{(a \beta)}^{(2)}(x),
\]

and they contain 27 Goldstone diagrams in total [9].

5. Conclusion

We have reviewed the symbolic programming package \( NC\) operators concentrating on the applications to many-body perturbation theory. We have shown that the package is capable to generate expansion terms up to the third-order RSPT and represent them in the irreducible tensor form by exploiting the angular momentum theory. On the basis that makes \( NC\) operators be multifaceted we hope that with minor modifications, if such are necessary at all, the package can be adapted to many other areas that apply the methods briefly considered in the present paper.

References

[1] Bochevarov A D and Sherrill C D 2004 J. Chem. Phys. 121 3374
[2] http://www.files.chem.vt.edu/chem-dept/valeev/software/sequant/sequant.html
[3] Derevianko A 2010 J. Phys. B: At. Mol. Opt. Phys. 43 074001
[4] http://homepage.cem.itesm.mx/lgomez/quantum/
[5] Žitko R 2011 Comp. Phys. Commun. 182 2259
[6] Racah G 1942 *Phys. Rev.* **61** 186
[7] Racah G 1942 *Phys. Rev.* **62** 438
[8] Fano U and Racah G 1959 *Irreducible Tensorial Sets* vol 4 (New York: Academic Press)
[9] Juršénas R and Merkelis G 2010 *J. Math. Phys.* **51** 123512
[10] Juršénas R and Merkelis G 2011 *Cent. Eur. J. Phys.* **9** 751
[11] Fritzschke S 1997 *Comp. Phys. Commun.* **103** 51
[12] Gaigalas G, Fritzschke S and Fricke B 2001 *Comp. Phys. Commun.* **135** 219
[13] Fritzschke S, Inghoff T, Bastug T and Tomaselli M 2001 *Comp. Phys. Commun.* **139** 314
[14] Juršénas R and Merkelis G 2011 *At. Data Nucl. Data Tables* **97** 23
[15] Jucys A P, Levinson Y B and Vanagas V V 1960 *Mathematical Apparatus of the Theory of Angular Momentum [in Russian]* vol 3 (Gospolitnauchizdat)
[16] Varshalovich D A, Moskalev A N and Khersonskii V K 1975 *Quantum Theory of Angular Momentum [in Russian]* (Leningrad: Nauka)
[17] Jucys A P and Bandzaitis A A 1977 *Theory of Angular Momentum in Quantum Mechanics [in Russian]* (Vilnius: Mokslas)
[18] Lindgren I and Morrison J 1982 *Atomic Many-Body Theory* vol 13 (Springer Series in Chemical Physics)
[19] Judd B R 1963 *Operator Techniques in Atomic Spectroscopy* (New York: McGraw-Hill)
[20] Rudzikas Z and Kaniauskas J 1984 *Quasispin and Isospin in the Theory of Atom [in Russian]* (Vilnius: Mokslas)
[21] Kaniauskas J, Č Šimonis V and Rudzikas Z B 1987 *J. Phys. B: At. Mol. Opt. Phys.* **20** 3267
[22] Rudzikas Z 1997 *Theoretical Atomic Spectroscopy* (Cambridge: Cambridge Univ. Press)