Atomic Structure Studies Accounting for Quasispin Space

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The efficient evaluation and decomposition of many–electron matrix elements is one of the central requirements in atomic structure calculations. It often adjudicates on the precision of the computation which can be obtained for a given system. Apart from the (basic) electron configurations — as typically used for characterizing the atomic levels and processes — correlation effects need often to be considered to a very large extent in order to achieve a requested accuracy. — And although standard approaches like the multiconfiguration Dirac–Fock (MCDF) or many–body perturbation theory (MBPT) allow for a systematic investigation, their application is often limited by the effort in evaluating all of the matrix elements.

It is therefore desirable to accelerate and unify the computation of the many–electron matrix elements. Several approaches are known for evaluating these matrix elements for one– and two–particle operators between configuration state functions with any number of open shells [1]. One of the most widely–used computational schemes is due to Fano [2] which is based on the coefficients of fractional parentage (CFP).

Recently, a new approach was developed by Gaigalas, Rudzikas and Froese Fischer [3] to evaluate matrix elements, those non–diagonal with respect to configurations included. In this work, it was found that a number of difficulties with the traditional decomposition can be avoided by applying the concept of second quantization in a *coupled tensorial form*, based on the theory of angular momentum, quasispin formalism as well as Wick's theorem. Instead of using CFP coefficients, this approach is based on the reduced coefficients (subcoefficients) of fractional parentage (RCFP) and the completely reduced matrix elements of the standard operator $W^{(k_q k_j)}$. The double tensor $W^{(k_q k_j)}$ is defined as the tensorial product of two second quantization operators $a^{(qj)}$, where q denotes its rank in quasispin space,

$$W^{(k_q k_j)}_{m_q m_j} = \left[a^{(qj)} \times a^{(qj)} \right]^{(k_q k_j)}_{m_q m_j} . \qquad (1)$$

Such an operator plays exceptional role in atomic spectroscopy, because all matrix elements of any physical operator may be expressed in terms of the reduced matrix elements of this operator or the sums of their products.

The tensorial structure of this operator then enables us to apply the Wigner–Eckart theorem in $Q-$space also to its matrix elements

$$\left(j^N\ \alpha QJM_Q||\,W^{(k_qk_j)}_{m_q}\,||j^{N'}\ \alpha'Q'J'M'_Q\right)$$

$$= \ -[Q]^{-1/2}\begin{bmatrix} Q' & q & Q \\ M'_Q & m_q & M_Q \end{bmatrix}\left(j\ \alpha QJ|||\,W^{(k_qk_j)}\,|||j\ \alpha'Q'J'\right), \qquad (2)$$

from which we find immediately the relation between the submatrix elements and the *completely reduced* matrix elements of the operator $W^{(k_qk_j)}$. The latter one $\left(j\ \alpha QJ|||\,W^{(k_qk_j)}\,|||j\ \alpha'Q'J'\right)$ is independent of the occupation number N of the corresponding subshell state; the occupation is incorporated into M_Q and, thus, occurs on the right–hand side as projection of the quasispin only within the Clebsch–Gordan coefficient.

Thus, by applying the quasispin method to the calculation of matrix elements of physical operators between different subshell states, we can exploit the completely reduced matrix elements. In practise, this approach has the advantage that the *internal* tabulations become much smaller when compared to other schemes, particularly if subshells with $j \geq 7/2$ are involved.

As was mentioned above the RCFP and the reduced matrix elements of the operator $W^{(k_qk_j)}$ are the main quantities in the approach [3]. The properties and tables of RCFP were discussed by Gaigalas, Fritzsche and Rudzikas [4]. The tables of reduced matrix elements of the operator $W^{(k_qk_j)}$ neither be compiled nor published yet. Therefore, the intention of our present work is to provide a tabulation of these quantities for all subshells with $j \leq 9/2$.

These completely reduced matrix elements are obtained from the relationship between the completely reduced matrix elements of $W^{(k_qk_j)}$ and RCFP and the tables of RCFP by using the RACAH package [5] which was extended to the reduced coefficients of fractional parentage.

A number of properties are known for the completely reduced matrix elements of operator $W^{(k_qk_j)}$. The numerical values of these quantities were checked making use of the properties mentioned above.

Our work has been encouraged in particular by systematic MCDF studies on open $d-$ and $f-$shell elements [6, 7, 8] where correlation effects force to include single, double, and (sometimes even) triple excitations within large active spaces. Additional motivation arises from the recent experiments and the discovery of heavy and superheavy elements ($Z > 95$) for which excitations into $j = 9/2$ subshells are inevitable.

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