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Computer Physics Communications 148 (2002) 349–351

Computer Physics
Communications

www.elsevier.com/locate/cpc

Pure spin-angular momentum coefficients for non-scalar one-particle operators in jj -coupling [☆]

G. Gaigalas ^a, S. Fritzsche ^{b,*}

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

^b *Fachbereich Physik, Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany*

Received 25 March 2002; accepted 24 May 2002

Abstract

A revised program for generating the spin-angular coefficients in relativistic atomic structure calculations is presented. When compared with our previous version [G. Gaigalas, S. Fritzsche and I.P. Grant, *Comput. Phys. Comm.* 139 (2001) 263], the new version of the ANCO program now provides these coefficients for both, scalar as well as *non-scalar* one-particle operators as they arise frequently in the study of transition probabilities, photoionization and electron capture processes, the alignment transfer through excited atomic states, collision strengths, and in many other investigations.

The program is based on a recently developed formalism [G. Gaigalas, Z. Rudzikas and C.F. Fischer, *J. Phys. B* 30 (1997) 3747], which combines techniques from second quantization in coupled tensorial form, the theory of quasispin, and the use of *reduced* coefficients of fractional parentage, in order to derive the spin-angular coefficients for complex atomic shell structures more efficiently. By making this approach now available also for non-scalar interactions, therefore, studies on a whole field of new properties and processes are likely to become possible even for atoms and ions with a complex structure.

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NEW VERSION SUMMARY

Title of program: ANCO⁽²⁾

Catalogue identifier: ADQO

Program Summary URL: <http://cpc.cs.qub.ac.uk/summaries/ADQO>

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Catalogue identifier of previous version: ADOO [1]; title: ANCO

Authors of the original program: G. Gaigalas, S. Fritzsche and I.P. Grant

Does the new version supersede the previous one: Yes, apart from scalar one- and two-particle tensor operators, the program now supports also *non-scalar* one-particle operators \hat{A}^k for any rank $k > 0$

Licensing provisions: None

Computer for which the new version has been tested: IBM RS 6000, PC Pentium II, AMD Athlon K7

Installations: University of Kassel (Germany); Institute of Theoretical Physics and Astronomy (Lithuania)

[☆] This program can be downloaded from the CPC Program Library under catalogue identifier: <http://cpc.cs.qub.ac.uk/summaries/ADQO>

* Corresponding author.

E-mail address: s.fritzsche@physik.uni-kassel.de (S. Fritzsche).

Operating systems: IBM AIX 6.2.2+, Linux 7.1

Program language used in the new version: ANSI standard Fortran 90/95

Memory required to execute with typical data: 200 kB

No. of bits in a word: All real variables are parameterized by a selected kind parameter. Currently this parameter is set to double precision (two 32-bit words) for consistency with other components of the RATIP package [2]

No. of bytes in distributed program, including test data, etc.: 3 637 988

Distribution format: Compressed tar file

Keywords: Atomic many-body perturbation theory, complex atom, configuration interaction, effective Hamiltonian, multiconfiguration Dirac–Fock, photoionization, Racah algebra, reduced matrix element, relativistic, second quantization, spin-angular coefficients, tensor operators, transition probabilities, 9/2-subshell

Nature of the physical problem

The matrix elements of a one-electron tensor operator \hat{A}^k of (any) rank k with respect to a set of configuration state functions (CSF) $|\gamma_i J_i P_i\rangle$ can be written as $\sum_{ij} t_{ij}^k(ab) \langle a | \hat{A}^k | b \rangle$ where the *spin-angular coefficients* $t_{ij}^k(ab)$ are independent of the operator \hat{A}^k , i, j are CSF labels and a, b specify the interacting orbitals. A combination of second-quantization and quasispin methods has been utilized in order to derive and to obtain these angular coefficients for one-electron tensor operator of any rank [3]. Operators of non-scalar rank, $k > 0$, occur frequently, for instance, in the study of transition probabilities, photoionization and electron capture processes, alignment transfer, collision strengths, and elsewhere.

Reasons for the new version

The RATIP package [2] has been found an efficient tool during recent years, in order to exploit the (relativistic atomic) wave functions from the GRASP92 program [4] for the computation of atomic properties and processes. Apart from a more efficient set-up of the (Dirac–Coulomb–Breit) Hamiltonian matrix [5], the RATIP program now supports *large-scale* computations of transition probabilities within a *relaxed* orbital basis [6], Auger rates and angular-anisotropy parameters [7], and of several other quantities. For these properties, the spin-angular coefficients for scalar one- and two-particle operators are sufficient, as be obtained from the previous version of ANCO [1]. However, in order to extend the range of (possible) applications also to other processes such as the atomic photoionization, (radiative) electron capture, or photoexcitation and alignment studies, *non-scalar* one-particle operators will occur and need to be treated efficiently. With the presently revised version of ANCO, we provide the spin-angular coefficients for such operators, making use of the modern design of the RATIP package in Fortran 90/95 [8]. Similarly as for all previously implemented components of this package, the revised ANCO program facilitates the use of

large wave function expansions of several ten thousand CSF or even more in the future.

Summary of revisions

When compared with the previous CPC version of the ANCO program [1], the following modifications and (new) capabilities have been added:

- (1) The module `rabs_recoupling` has been enlarged to include further expressions from Ref. [9], i.e. Eqs. (14) and (19). These expressions are incorporated into the routines `recoupling_matrix_1p_shell` for calculating the recoupling matrix for the case of CSF with one open shell and into `recoupling_matrix_2p_shells` for CSF with two open shells, respectively. Moreover, the subroutine `recoupling_C_3` has been added to derive the C_3 coefficients, cf. [9, Eq. (17)].
- (2) Several procedures have been added also to the module `rabs_anco` to enable the user with a simple and direct access to the spin-angular coefficients. For example, the two routines `anco_calculate_csf_pair_1p` and `anco_calculate_csf_matrix_1p` provide these coefficients for any one-particle operator with specified rank, either for a single pair of CSF or for a whole array of such functions, respectively. Both procedures make use of the subroutines `anco_one_particle_diag` for the diagonal matrix elements and `anco_one_particle_off` otherwise. In `anco_calculate_csf_matrix_1p`, the spin-angular coefficients are calculated for any rank $k \geq 0$ either for the whole matrix or for a sub-matrix with rows from (given) `row_low ... row_up` and columns from `col_low ... col_up`. While the procedure `anco_calculate_csf_pair_1p` returns `no_T_coeff` coefficients directly in the array `anco_T_list`, the coefficients of a whole CSF array are returned in the derived data structure `anco_pair_list`; see the header of the module `rabs_anco` for further details.
- (3) The definition and set-up of properly derived data types in [1] has definitely helped facilitate the data exchange between different components of the RATIP package. These data structures have been used also for extending the ANCO program. For the one-particle coefficients, for example, the derived type

```

type :: anco_T_coeff
  integer      :: nu
  type(nkappa) :: a, b
  real(kind=dp) :: T
end type anco_T_coeff

```

were introduced already in our previous version, where we used `nu = 0` to designate the scalar interaction. The integer `nu` now indicates simply the rank of the (one-particle) tensor. In further applications of RATIP, therefore, these coefficients can be easily accessed if the module `rabs_anco` is properly used by the additional code.

- (4) A few minor changes are made also in the (interactive) dialog which controls the program as well as for the printout of the spin-angular coefficients. One additional question in the dialog:

Generate one-electron angular coefficients
for non-scalar interactions?

can first be answered with n or N—if non-scalar coefficients are not requested. If answered by y or Y, the additional question:

Generate GRASP92-like d coefficients
for non-scalar interactions?

arise and help the user to select GRASP92-like $d_{ab}^k(rs)$ coefficients, such as previously obtained from the MCT component of GRASP, or ‘pure’ angular coefficients (as utilized within RATIP). Finally, the prompt

Enter the rank of the tensor:

requests the user to specify the rank of the one-particle operator.

- (5) As previously, the ANCO program generates two output files; while the .sum ANCO summary file provides a short summary of the computations, the spin-angular coefficients and all necessary quantum numbers for their classification are stored in the .vnu file. The format for printing the $d_{rs}^k(ab)$ and $t_{rs}^k(ab)$ is very similar to each other, apart from the sorting process which is used in GRASP92 [4] and which is not done by ANCO.

As before, the source code of the ANCO component is distributed together with the source of all other components of RATIP in order to facilitate the installation and to save the user from additional adaptations to be made. The whole package is provided as a compressed `Ratip_anco.tar.Z` archive file. On a UNIX (or any compatible) system, the two commands `uncompress Ratip_anco.tar.Z` and `tar xvf Ratip_anco.tar` will reconstruct the file structure. The obtained `ratip` root directory then obtains the source code, the file `make-anco` for generating the executable `xanco` and the subdirectory `test-anco` for the test example. Details of the installation are explained also in the `Read.me` file in the `ratip` root directory.

Restrictions onto the complexity of the problem

For all subshells with $j \geq 11/2$ (i.e. $h_{11/2}$ -, i -, ... electrons), the maximal number of *equivalent electrons* is restricted to two.

Typical running time

This strongly depends on the system and the size of the wave function expansion to be considered. Our test case, which is distributed with the code in the subdirectory `test-anco`, required 32 s on a 1400 MHz AMD Athlon K7/1400T. Typically, ANCO calculates about 10,000 angular coefficients per second.

Unusual features of the program

ANCO has been designed as component of the RATIP package [2] for calculating a variety of *relativistic atomic transition and ionization properties*. Owing to the careful use of allocatable and `pointer` arrays, there is (almost) no restriction on the size or any dimension of the “physical problem” apart from the computer resources themselves.

References

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