



CESD99 – A new version to represent atomic wave functions in a determinant basis [☆]

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Abstract

Determinant expansions of atomic wave functions have several advantages for calculating transition probabilities and cross sections. For instance, such a representation can easily be applied to rather a large number of transition operators and also in order to include rearrangement effects of the bound-state density following the excitation or the decay of an atomic state. In practice, the *rearrangement* of the electron density is most simply taken into account if the variation of the initial and final state wave functions is carried out separately in studying transition or ionization processes. Of course, such a computational procedure yields sets of one-electron orbitals which are not quite orthogonal to each other and which do require special care in evaluating the (many-electron) transition matrix.

For relativistic wave functions of the atomic structure package GRASP92 [F.A. Parpia, C.F. Fischer, I.P. Grant, CPC 92 (1996) 249], a determinant representation of the atomic states is obtained by the CESD97 program [S. Fritzsche, I.P. Grant, CPC 103 (1997) 277]. This program performs a complete expansion of symmetry-adapted functions and has been found useful in a number of applications. For accurate transition probability studies, however, often large wave function expansions of several ten or even hundred thousand determinants are required which cannot be handled by CESD97 due to the demand on memory and computing time. Further difficulties were caused by the tight binding of both GRASP92 and CESD97 to the IBM XL Fortran standard. To overcome these difficulties and to facilitate the transfer to other architectures, CESD97 has entirely been rewritten according to the ANSI standard Fortran 90/95. The new version, CESD99, considerably improves the efficiency of large computations and, now, enables wave function expansions based on several (hundred) thousand determinants. The conversion to Fortran 90/95 is considered as major step to render the CESD program ready to use for systematic investigations of open-shell atoms. CESD99 is part of the RATIP package for the calculation of relativistic atomic transition and ionization properties and will be distributed within this framework [S. Fritzsche, C.F. Fischer, C.Z. Dong, this volume]. © 2000 Elsevier Science B.V. All rights reserved.

NEW VERSION SUMMARY

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

Title of program: CESD99

Catalogue number: ADLG

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland. Users may obtain the program also by down-loading a tar-file `ratip99.tar` from our home page at

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the University of Kassel (<http://www.physik.uni-kassel.de/fritzsche/programs.html>)

Catalogue identifier of previous version: ADFW [1]; title: CESD97

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

Does the new version supersede the previous one

Yes, beyond several modifications related to the internal data representation (see below), the program has entirely been re-written according to the ANSI standard Fortran 90/95 [2]. By using derived data types, modules as well as a dynamic storage management for most arrays, the new version enables sizeable wave function expansions even on present-day PCs.

Licensing provisions: None

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

Installations: University of Kassel (Germany)

Operating systems: IBM AIX 4.1.2+, Linux 6.1

Program language used in the new version: ANSI standard Fortran 90/95; all language features which are considered as *obsolete* by this recent standard have been avoided completely

Memory required to execute with typical data: 2–20 MB

No. of bits in a word

All real variables are parameterized by a `selected kind parameter` and, thus, can easily be adapted to any required precision as supported by the compiler. Presently, the `kind` parameter is set to double precision (two 32-bit words); see Ref. [3] in this volume for details.

Peripheral used: Disk for input/output

No. of bytes in distributed program, including test data, etc.: 4943 716 (please note there is one file for the programs described in this paper and the one described in Ref. [3])

Distribution format: unencoded compressed tar file; see Ref. [3]

Keywords: Atomic, configuration, decoupling, determinant representation, multiconfiguration Dirac–Fock, relativistic

Nature of the physical problem

The atomic state functions (ASF) of the structure program GRASP92 [4] are expanded into a determinant basis.

Reasons for the new version

Accurate atomic structure calculations often require large wave function expansions which are based on several thousand or even

tens of thousand configuration state functions (CSF). While large expansions became recently more and more in use for studying level energies and fine-structures of open-shell atoms [5,6], such wave function expansions are much less supported if transition or ionization properties need to be studied. The shortcome of the presently available programs first of all concerns the demand on memory and CPU time if expansions of more than a few thousand CSF are involved. In order to increase the efficiency of our previous implementation, CESD97 [1] has completely been rewritten. CESD99, the new version, now supports wave function expansions up to several hundred thousands determinants and still requires only reasonable resources. Two further reasons for providing a revised version concerned the tight binding of CESD97 to the IBM RS 6000 architecture and a previous limitation that each (single) CSF could has just a maximum of five open subshells. The strong dependence of CESD97 on the IBM standard followed the “lines” of GRASP92 [4] and made it difficult in the past to transport these programs to other environments. By applying the ANSI standard Fortran 90/95, CESD99 is now easy to “move” and has been tested on several platforms. In addition, to make CESD99 capable for the investigation of Auger and inner-shell processes, the maximal number of open subshells has been increased to 9 for each CSF.

Summary of revisions

Important modifications and new capabilities of CESD99, if compared with the previous CPC version [1], are:

(1) Derived data types and allocatable respective pointer arrays are consistently used for defining appropriate data structures. For example, derived types are defined to keep all information about a single CSF and a single determinant together; these types are then applied, in turn, for defining data structures of a complete CSF or determinant basis. Further derived types are related to (complete) sets of quantum numbers, the representation of eigenvectors, and many others. The choice of properly derived types facilitates the data exchange between different components of the RATIP package (see [3]); such components deal with the computation of Auger rates and photoionization cross sections in the multiconfiguration Dirac–Fock model and are currently transformed to the present standard.

(2) Dynamic allocation is applied to (almost) all arrays and is used with assumed-shape assignments in order to ensure that just the required memory is needed.

(3) The internal representation of the occupation numbers 0 and 1 of the one-electron orbitals in the determinant basis. These occupation numbers are now held *bitwise* within integers and are treated by the (intrinsic) bit manipulation procedures of Fortran 90/95. Thus, the required memory to store the full basis has been reduced either by a factor of 8 or even 32, if compared with CESD97, dependent on the support of the (non-standard) `integer*1` data type by the compiler previously used.

(4) To deal with large CSF lists from GRASP92 [4], a fast comparison of symmetries and occupation numbers is required in order to ascertain whether a given determinant is already part of the expansion or not. A *reverted* search procedure in which the most recently appended determinant in the expansion is considered first, has been found useful and has reduced run times by a factor of 4 to 10. The

computing time now increases approximately linear with the number of CSF in the computation while a considerable enhancement in CPU time was found previously.

(5) Even though the CESD99 expansion (.xpn) file has still ASCII format to facilitate the file transfer from one system to another, it is now written in a more compact form by applying the bitwise representation of the occupation numbers within a suitable number of standard integers.

(6) In contrast to previous implementations, CESD99 does not depend on links to GRASP92 procedures. All subprograms which are required for loading and handling the GRASP92 data files have been adapted to the new ANSI standard and incorporated into the package.

The distribution of the CESD99 program will be explained together with the revised set-up of the RATIP package in Ref. [3].

(7) A few minor modifications concern the interactive dialog and the printout of intermediate results if the corresponding flags were set.

Restrictions onto the complexity of the problem

Like for GRASP92, the number of electrons in subshells with $j \geq 9/2$ is restricted to two. For those large one-electron angular momenta, j , additional quantum numbers would be needed to classify the corresponding antisymmetric subshell states uniquely. The present version now allows a total of 9 open subshells for each CSF.

Typical running time

This strongly depends on the atomic system and the size of the wave function expansion as applied to the GRASP92 package. In addition to the number of CSF in the expansion, the CPU time depends on the

set of peel shells. Typically, expansions of 100–300 CSF per minute have been observed in many computations along different isoelectronic sequences. For the test cases, which are distributed with the code in the subdirectory `test-cesd99`, CPU times of 10 respective 12 minutes were required on a 266 MHz Pentium II processor.

Unusual features of the program

CESD99 is one component of the RATIP package (cf. [3]) for calculating *relativistic atomic transition and ionization properties*. This package has been developed to extend the application of GRASP92 wave functions. CESD99 now exploits, together with REOS99 [3], the ANSI Fortran 90/95 standard to enable the maintenance of the package into the next century. Owing to the careful use of `allocatable` and `pointer` arrays there is (almost) no restriction on the size or any dimension of the problem apart from the computers themselves.

References

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