Computer Physics Communications 128 (2000) 635, 636

Computer Physics Communications

www.elsevier.nl/locate/cpc

The MCHF atomic-structure package

Charlotte Froese Fischer

Department of Computer Science, Box 1679 B, Vanderbilt University, Nashville, TN 37235, USA

Received 10 December 1999

Abstract

The programs, as described in *Computational Atomic Structure: An MCHF Approach* (C. Froese Fischer, T. Brage, and P. Jönsson, Institute of Physics (Bristol, 1997)) are collected into an atomic structure package. Included with the package are test examples with complete output of results. Also included are executable binaries for the Intel Linux operating system. The programs have previously been published separately except for a simple continuum CMCHF program with one continuum channel and associated photoionization program that are unpublished.

Keywords: Atomic structure; Multiconfiguration Hartree–Fock (MCHF); Configuration interaction; Correlation; Bound states; *LS* coupling; Breit–Pauli; Isotope shifts; Hyperfine interactions; Oscillator strengths; Transition rates; Autoionization; Photoionization

CPC Program Library index: 2.1 Atomic Physics. Structure and Properties

PROGRAM SUMMARY

Title of program: ATSP_MCHF; *version number:* 1.00

Catalogue identifier: ADLY

Program summanry URL: http://cpc.cs.qub.ac.uk/summaries/ADLY

Distribution format: gzipped tar file

References in CPC to previous version:

1. C. Froese Fischer, Comput. Phys. Commun. 64 (1991) 369.
2. C. Froese Fischer, Comput. Phys. Commun. 64 (1991) 399.
3. C. Froese Fischer, B. Liu, Comput. Phys. Commun. 64 (1991) 406.
4. A. Hibbert, C. Froese Fischer, Comput. Phys. Commun. 64 (1991) 417.
5. C. Froese Fischer, Comput. Phys. Commun. 64 (1991) 431.
6. A. Hibbert, R. Glass, C. Froese Fischer, Comput. Phys. Commun. 64 (1991) 455.
7. C. Froese Fischer, Comput. Phys. Commun. 64 (1991) 473.
8. C. Froese Fischer, M.R. Godefroid, A. Hibbert, Comput. Phys. Commun. 64 (1991) 486.
9. C. Froese Fischer, M.R. Godefroid, Comput. Phys. Commun. 64 (1991) 501.
10. C. Froese Fischer, Tomas Brage, Comput. Phys. Commun. 74 (1993) 381.
11. P. Jönsson, C.-G. Wahlström, C. Froese Fischer, Comput. Phys. Commun. 74 (1993) 399.
12. C. Froese Fischer, L. Smentek-Mielczarek, N. Vaeck, G. Miecznik, Comput. Phys. Commun. 74 (1993) 415.

Catalogue identifier of previous version: ABZU, ABZV, ABZW, ABZX, ABZY, ABZZ, ACBA, ACBB, ACLD, ACLE, and ACLF

Authors of previous version: C. Froese Fischer, B. Liu, A. Hibbert, R. Glass, M.R. Godefroid, Tomas Brage, P. Jönsson, C.-G. Wahlstrom, L. Smentek-Mielczarek, N. Vaeck, and G. Miecznik

Does the new version supersede the original program?: no

Computer for which the new version is designed and others on which it has been tested:

0010-4655/00/$ – see front matter
PII: S0010-4655(00)00009-6

Computers: SUN Ultra 1, Pentium-based PCs

Installations: Vanderbilt University, Nashville, TN 37235, USA

Operating systems or monitors under which the new version has been tested: Sun UNIX OS 5.2, and LINUX 2.2.10

Programming language used in the new version: FORTRAN 77

Memory required to execute with typical data: 64 000 KBytes

Peripherals used: terminal, disk

No. of bits in a word: 32

No. of processors used: 1

Has the code been vectorised or parallelized?: no

No. of bytes in distributed program, including test data, etc.: 2 299 247 bytes

CPC Program Library subprograms used: none

Nature of physical problem
This package determines the energy and associated wave functions for states of atoms and ions in the multiconfiguration Hartree–Fock (MCHF) approximation. Once radial functions have been determined, relativistic effects may be included through the diagonalization of the Breit–Paul Hamiltonian. Given a wave function, various atomic properties can be computed such as E1, E2, ... , M1, M2, ... transitions between *LS* or *LSJ* states, isotope shift constants, and hyperfine interactions. Autoionization and simple photoionization calculations can also be performed.

Method of solution
Wavefunctions are obtained using variational methods leading to systems of differential equations for radial functions and the matrix eigenvalue problem for expansion coefficients of configurations states. The radial functions are obtained using finite difference methods.

Reason(s) for the new version
The previous version was published as a series of programs, each associated with specific co-authors. In this, the entire package is collected into a directory structure with a `make_atsp` script that illustrates how the application can be generated. Intel PC executables are provided for PC users who do not have a FORTRAN compiler. Included also is a simple continuum MCHF program [1] with one open channel and an associated photionization program. Use of the program is described in the book [2].

Summary of revisions
Previously published programs together with two unpublished programs have been collected and placed either in `lib_src` or `atsp_src` source directories that include makefiles for the different objects. A `test_run` directory has been added with script files that, when executed produce, results that can be checked with similar information in the `results` directory. The make directory contains a `make_atsp` that will make the applications on many platforms.

Restrictions on the complexity of the problem
The restrictions are those of the previous publications. The README file explains the different parameter statements that determine the size of the problem. Many restrictions may be relaxed by changing the value of parameter statements, but the restriction of a maximum of 5 open shells is no easily overcome. A limited amount of non-orthogonality of orbitals is allowed.

Typical running time
A single and double replacement expansion from the $2s^2 2p^2\ ^3P$ term of carbon to the orbitals $2p, 3s, 3p, 3d$ leading to 69 configuration states, required a total of 3.0 seconds for both angular and radial calculations on a SUN Ultra 1.

Unusual features of the program
Intel PC executables are provided for those without a FORTRAN compiler running the LINUX operating system. Background theory for the execution of the various applications is presented in a book [2] with selected examples. A limited amount of non-orthogonality between orbitals is allowed in the calculation of atomic properties.

References

[1] C.F. Fischer, J. Xi (unpublished).
[2] C.F. Fischer, T. Brage, P. Jönsson, Computational Atomic Structure: An MCHF Approach (Institute of Physics, Bristol, 1997).