BSR: B-spline atomic R-matrix codes

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Abstract

BSR is a general program to calculate atomic continuum processes using the B-spline R-matrix method, including electron-atom and electron-ion scattering, and radiative processes such as bound-bound transitions, photoionization and polarizabilities. The calculations can be performed in LS-coupling or in an intermediate-coupling scheme by including terms of the Breit-Pauli Hamiltonian.

NEW VERSION SUMMARY

Title of program: BSR

Catalogue identifier: XXXX

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

Computers on which the program has been tested: Microway Beowulf cluster; Compaq Beowulf cluster; DEC Alpha workstation; DELL PC

Operating systems under which the new version has been tested: UNIX , Windows XP

Programming language used: FORTRAN 95

Memory required to execute with typical data: Typically 256 – 512 Mwords. Since all the principal dimensions are allocatable, the available memory defines the maximum complexity of the problem.

No. of bits in a word: 8

No. of processors used: 1

Has the code been vectorized or parallelized?: no

No. of bytes in distributed program: 2 157 700

Peripherals used: scratch disk store; permanent disk store

No. of lines in distributed program, including test data, etc.: 69 970

Distribution format: gzip file

Nature of physical problem
This program uses the R-matrix method to calculate electron-atom and electron-ion collision processes, with options to calculate radiative data, photoionization etc. The calculations can be performed in LS-coupling or in an intermediate-coupling scheme, with options to include Breit-Pauli terms in the Hamiltonian

Method of solution
The R-matrix method is used [1,2,3].

References
 [1] P.G. Burke and K.A. Berrington, Atomic and Molecular Processes: an *R*-matrix Approach (Institute of Physics Publishing, Bristol,1993).
[2] P.G. Burke and W.D. Robb, Adv. At. Mol. Phys. 11 (1975) 143.
[3] K.A. Berrington, W.B. Eissner and P.H. Norrington, Comput. Phys. Commun. 92 (1995) 290.

LONG WRITE-UP

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