

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.

PACS: 34.80Dp; 34.80Kw; 32.80Fb; 31.15Ar

Keywords: Electron atom scattering; Electron ion scattering; Photoionization; Oscillator strengths; Polarizability; *R*-matrix; *B*-splines

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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References