

DBSR: Dirac-based fully-relativistic B-spline atomic R-matrix codes

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Abstract

DBSR 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 are performed in *jj*-coupling scheme using the Dirac-Coulomb-Breit Hamiltonian.

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

New version program summary

Title of program: DBSR

Catalogue identifier: XXXX

Program summary URL: xxxxxxxx

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

Computers on which the program has been tested: Microway Beowulf cluster; ASUS PC; Apple MAC; Stampede supercomputer

Operating systems under which the new version has been tested: UNIX , Windows 8

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 lines in distributed program, including test data: xxx

No. of bytes in distributed program, including test data: xxx

Peripherals used: scratch disk store; permanent disk store

Distribution format: tar.gz

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 are performed in *jj*-coupling using the Dirac-Coulomb-Breit Hamiltonian.

Method of solution

The *R*-matrix method is used [P.G. Burke, *R*-Matrix Theory of Atomic Collisions, Springer-Verlag, Berlin, Heidelberg 2011]

LONG WRITE-UP

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Acknowledgements

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