The ATSP2K and GRASP2K Multiconfiguration Atomic Structure Program Packages

Per Jönsson[*,1] **Gediminas Gaigalas**[†], **Michel Godefroid**[‡], **Jacek Bieroń**[**], **Charlotte Froese Fischer**[‖],

[*] Group for Materials Science and Applied Mathematics, Malmö University, Malmö, Sweden
[†] Institute of Theoretical Physics and Astronomy, A. Gostauto 12, Vilnius LT-01108, Lithuania
[‡] Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles B 1050 Brussels, Belgium
[**] Instytut Fizyki imienia Mariana Smoluchowskiego, Uniwersytet Jagielloński, Poland
[‖] Atomic Physics Division, National Institute of Standards and Technology, Gaithersburg, Maryland, USA

Synopsis The ATSP2K and GRASP2K program packages for large scale atomic calculations are presented. A number of applications are given to illustrate the potential and restriction of the packages.

ATSP2K [1] and GRASP2K [2, 3] are two program packages designed primarily for large scale atomic calculations based on multiconfiguration methods. The ATSP2K is non-relativistic and adds relativistic corrections in the Breit-Pauli approximation. GRASP2K is fully relativistic. By extensive use of default options together with a naming convention for the files, the packages are user friendly with little input data for the typical cases. The program packages are well documented [4] and comprehensive user manuals are available [3]. In both packages the wave functions are given as expansions over configuration states functions that are built from antisymmetrized and coupled products of one-electron orbitals. The expansion coefficients and radial parts of the orbitals are determined in the self-consistent field procedure. Once one-electron orbitals are known configuration interaction can be performed, where higher order interactions such as the Breit interaction and quantum electrodynamic effects are added perturbatively. Parallel processing using MPI allows large scale computing.

Both packages implement a biorthonormal transformation method that permits initial and final states in a transition array to be optimized separately, which, in many cases, leads to more accurate values of the resulting rates [5]. In addition to energy structures and transition rates a number of other properties such as hyperfine structure, isotope shift with relativistic corrections to the normal and specific mass shift operators [6] and splittings in external magnetic fields can be computed. New developments of the biorthonormal transformation methods allow general matrix elements between non-orthogonal states to be computed making an interesting link to continuum functions.

We present results for a number of systems and properties to illustrate the potential and restriction of the packages. Among the properties are transition energies, hyperfine structures and isotope shifts in the boron-isoelectronic sequence, transition rates for nitrogen-like ions, Landé g_J factors and splittings in external fields for neon-like ions.

References

[1] C. Froese Fischer, G. Tachiev, G. Gaigalas, and M R. Godefroid 2007 *Comput. Phys. Commun.* **176** 559

[2] P. Jönsson, X. He, C. Froese Fischer, and I.P. Grant 2007 *Comput. Phys. Commun.* **177** 597

[3] P. Jönsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, and I.P. Grant 2013 *Comput. Phys. Commun.*, at press

[4] C. Froese Fischer, T. Brage, P. Jönsson 1997 *Computational Atomic Structure*, IoP Publishing

[5] J. Olsen, M. Godefroid, P. Jönsson, P.Å. Malmqvist and C. Froese Fischer 1995 *Phys. Rev. E* **52** 4499

[6] C. Nazé *et al* 2013 *Comput. Phys. Commun.*, at press

[1] E-mail: per.jonsson@mah.se