1. Introduction

Over the past decades, a number of general computer codes have been developed to generate accurate data for electron and photon collisions with atoms and molecules. The *R*-matrix technique (Burk and Robb 1975) is often the method of choice, as illustrated in the compilation volume by Burke and Berrington (1993) and the recent comprehensive textbook of Burke (2011). The general *R*-matrix package RMATRX-I (Berringtin et al 1995) remains the most frequently used publicly available code for atomic and ionic targets. Other packages are around, such as the unpublished code RMATRX-II, with improved efficiency of the angular-momentum algebra; the parallelized version PRMAT (Sunderland et al 2002); an alternative version of RMATRX-I (http://amdpp.phys.strath.ac.uk/rmatrix/)] with the possibility of including radiative damping; and the intermediate-energy R-matrix code IERM (Burke and Scott 1996). The fully relativistic DARC package (unpublished but widely used) has predominantly been applied to highly ionized targets (Ait-Tahar 1996), but a Dirac-based R-matrix with pseudo-states (DRMPS) was described by Badnell (2008) and successfully applied to one-electron targets. However, we are not aware of follow-up applications since the proof-of-principle publication.

One of the principal ingredients of the above-mentioned programs is a single set of orthogonal one-electron orbitals, with one subset being used to construct the target states in multi-configuration expansions and the other one being employed to represent the scattered projectile. This structure simplifies the setup of the matrices and allows for the development of efficient computer programs. On the other hand, it often leads to three major problems when the current suite of codes is applied to truly complex targets: i) difficulties in describing all target states of interest to sufficient accuracy; ii) the possible occurrence of unphysical structures, so-called ”pseudo-resonances”, when an attempt is made to address the former problem; and iii) numerical difficulties due to an ill-conditioned orthogonalization procedure and the need to modify the so-called “Buttle corrections”.

Given the success of the R-matrix method for atomic structure and collision processes, it is not surprising that many modifications of the general idea and improved algorithms have been suggested since the original programs were published. These include the eigenchannel formulation (Fano and Lee 1973), a different choice of basis functions (Plummer and Noble 1999), particularly targeted to eliminate or reduce the sometimes problematic Buttle correction (Bartschat et al 1996, Gorczyca and Badnell 1997), and specific recipes to avoid the pseudo-resonance problem [Gorczyca et al 1995, Bartschat 1998). Also, the R-matrix Floquet approach (Burke et al 1991) and a truly time-dependent formulation (Burke amd Burke 1997, van der Hart et al 2007) allow for the treatment of strong-field short-pulse laser−atom interactions.

The BSR code (Zatsarinny 2006) is another implementation of the *R*-matrix method with two significant innovations compared to the existing codes:

- the non-orthogonal orbitals can be used to represent both the bound and continuum one-electron orbitals;
- a set of *B*-Splines defines the *R*-matrix basis functions.

The use of non-orthogonal bound orbital sets generally allows for significantly improved descriptions of the target states. Since they can be optimized in separate calculations, a high level of accuracy can be achieved with compact configuration interaction expansions. Regarding the close-coupling expansion of the total collision wavefunction, it should be noted that certain (N+1)-electron bound configurations must often be included to compensate for orthogonality constraints imposed on the continuum orbitals. However, it can be difficult to keep the expansion fully consistent, and any inconsistency may lead to

pseudo-resonance structure. No longer forcing orthogonality between the continuum and the bound orbitals avoids the introduction of these (N +1)-electron terms and thus may drastically reduce the pseudo-resonance problem.

Non-orthogonal orbital sets have been avoided for a long time, because the most time-consuming part of atomic structure calculations is connected with the angular integrations in constructing the hamiltonian matrix elements. After a set of efficient general codes was developed for this task for fully orthogonal orbitals and with some restricted non-orthogonality (Hibbert and Froese Fischer 1991), it became possible to automate, to a large extent, this part of the inner-region problem. A key step for the present approach is a set of efficient codes, developed by Zatsarinny and Froese Fischer (1999), for dealing with non-orthogonal orbital sets in a general way.

The choice of *B*-splines as basis functions, introduced to atomic structure calculations around 1980, is advantageous due to their excellent numerical approximation properties (see review by Bachau et al 2001). B-splines are bell-shaped piecewise polynomial functions of order k_s (degree $k_s - 1$), defined by a given set of points in some finite radial interval. There is great flexibility in the choice of the radial grid in a *B*-spline basis, and machine accuracy may be achieved with simple Gaussian quadratures. Finite-difference algorithms are avoided and well-established Linear Algebra packages are used instead.

Since the characteristic feature of the *B*-spline method is the solution of the Schrödinger or Dirac equation within a box, which is very similar to the inner region in the *R*-matrix method, *B*-splines are rightfully expected to be very effective in forming the *R*-matrix basis. Also, since *B*-splines form an effectively complete basis on the interval spanned by the knot sequence, no Buttle correction to the *R*-matrix elements is required. The use of *B*-splines as the *R*-matrix basis set was first outlined by van der Hart (1997), who applied the method to e−H scattering and obtained excellent agreement with existing benchmark results. Further significant progress in the method was achieved by Zatsarinny and Froese Fischer (2000), who developed a general non-relativistic computer code and applied it to photo-ionization of lithium, by Zatsarinny and Bartschat (2004), who produced the semi-relativistic (Breit-Pauli) extension. The BSR code was extensively tested for truly complex systems, including electron scattering on the noble gases, where considerable improvement in comparison to result of standard *R*-matrix calculations was obtained. We applied the code to many problems, both for benchmarking purposes and to assist colleagues in need of atomic data for various modeling purposes. Later, the BSR code was parallelized and extended to treat the electron-impact ionization in the continuum pseudo-state approach (Zatsarinny and Bartschat 2011), including the ionization plus excitation processes. Finally, field-free and dipole matrices generated by the method have been successfully combined with an efficient Arnoldi-Lanczos time-propagation scheme to treat intense attosecond laser interactions with complex targets such as Ne (Guan et al 2007) and Ar (Guan et al 2008).

The present paper describes a fully relativistic DBSR version based on the Dirac-Coulomb Hamiltonian. This code was first presented in 2008 for e-Cs collisions (Zatsarinny and Bartschat 2008) and since has been tested extensively for other heavy targets such as Kr, Xe, Au, Hg and Pb. We successfully overcame several roadblocks, including the appearance of spurious pseudostates in the spectrum of the Dirac-Coulomb Hamiltonian by employing B-spline bases of different order for the large and small components of the orbitals – in hindsight a simple but very effective solution (Froese Fischer and Zatsarinny 2009).

Both BSR and DBSR codes deal only with the inner-region problem, while the final step in the calculation requires the solution of the scattering problem in the external region, matching the solutions at the boundary ($r=a$). Once the *R*-matrix has been constructed, no further changes are required. Hence, any

improvements achieved in solving the outer-region problem, through packages such as STGF (Badnell 1999) or FARM (Burke and Noble 1995), can be taken advantage of immediately. Also, the calculation of bound states and the reconstruction of the wavefunction, as needed for the treatment of photoionization and photodetachment processes, proceeds along the same lines as in the standard implementations.

The write-up is organized as follows. In the next section we will briefly summarize the most important aspects of the *R*-matrix theory. The general features of the present DBSR complex are given in section 3, while each program in DBSR is then described in detail in Sections 4-11. Section 12 presents the libraries, common to all programs, including the Dirac *B*-spline library DBS, which is the key part of the present implementation. Additional program utilities, which can be used for preparing and processing input/output data, are given in Section 13, and finally Section 14 describes the test runs.

Unless otherwise specified, all quantities are expressed in atomic units.