Benchmark calculations for electron collisions with complex atoms

Oleg Zatsarinny and Klaus Bartschat
Department of Physics & Astronomy, Drake University, Des Moines, IA 50311, USA

E-mail: oleg.zatsarinny@drake.edu

Abstract. We report on a further extension of the B-spline R-matrix (BSR) method based on the continuum pseudostate approach. A new parallelized version of the BSR code is intended to carry out large-scale R-matrix with pseudostates calculations and to provide converged (with respect to the number of coupled states) results for electron impact excitation of individual target states. The pseudostate approach also provides a fully nonperturbative scheme for electron-impact ionization, including simultaneous ionization plus excitation processes. Illustrative examples are given for He, Ne, and Ar excitation and ionization, including fully-differential (energy and angles) cross sections. The BSR code is also being used to generate extensive datasets for plasma and astrophysical applications.

1. Introduction
Over the past decade, we have developed a highly flexible B-spline R-matrix (BSR) method [1] that has some advantages compared to the standard R-matrix (close-coupling) approach. The two essential refinements are (i) the removal of orthogonality restrictions, which allows for the use of nonorthogonal orbital sets to represent both the bound and continuum one-electron orbitals, and (ii) the use of B-splines as a universal and effectively complete basis to generate the R-matrix functions. These features allow us to achieve a high accuracy in the target description, as well as a truly consistent description of the scattering system. The BSR code was successfully applied to many problems of electron collisions from atoms and ions, and often considerable improvement was obtained in comparison to previous calculations. Many examples can be found in the recent topical review [2]. Special emphasis is placed on complex, open-shell targets, for which the method has proven very successful in reproducing, for example, a wealth of near-threshold resonance structures.

As the next step, we extended the BSR complex to the fully relativistic Dirac scheme (DBSR). The DBSR code retains all the advantages of the previous semi-relativistic version, including its generality as an all-electron code and the flexibility associated with the use of nonorthogonal orbital sets. The application of the fully relativistic scheme allowed us to obtain, for the first time, close agreement with experiment for electron scattering from such heavy atoms as Cs, Hg, Au, Pb, Kr and Xe (see references in review [2]).

During the past three years we developed parallel versions of our BSR and DBSR codes, which are intended to carry out large-scale R-matrix with pseudostates (RMPS) calculations and hence provide converged results for electron impact excitation of individual target states. The close-coupling expansion in our recent e-Ne calculations [3], for example, includes 457 target states, with the lowest 87 states representing the bound spectrum and the remaining 370 the ionization continuum. The
results reveal dramatic reductions of the predicted excitation cross sections at intermediate energies due to a strong influence of coupling to the target continuum, and they raise questions about the absolute normalization in the existing measurements.

With the pseudostate approach and the projection technique, the BSR code is also able to treat electron-impact ionization processes, including ionization with excitation, in a fully non-perturbative framework. As an example, we obtained, for the first time, excellent agreement with the directly measured experimental cross section ratios for ionization leaving the residual He$^+$ ion in either the 1s ground state or the $n = 2$ excited states [4]. In contrast to other methods, our approach is an all-electron \textit{ab initio} formalism that, in principle, can be applied to any many-electron target. Illustrative examples are selected from recent calculations of electron scattering from Ne and Ar atoms, including the detailed prediction of fully differential cross sections [5].

2. The pseudostate approach

The importance of coupling to highly excited states and the continuum has long been recognized, but the numerical implementation provides a major challenge. With the advancement of computational power over the past decade, the doorway has been opened to carry out large-scale numerical studies using the $R$-matrix with pseudo-states (RMPS) method. The RMPS idea was first pursued in the late 1960s by Burke, Gallagher and Geltman [6] in studying electron scattering from atomic hydrogen, with great success in reproducing the then available experimental data. In 1992, Bray and Stelbovics [7] demonstrated that convergence of the close-coupling expansion could be achieved for e-H collisions with a relatively small (~30) set of Laguerre pseudo-states. Subsequently, Bray and co-workers studied a wide range of excitation and ionization phenomena in quasi-one and quasi-two-electron targets with the convergent close-coupling method (CCC), obtaining impressive agreement with experiment [8].

The practical difficulty in the RMPS implication lies in orthogonalizing the continuum basis to the pseudo-state basis. The possible solution for this problem was suggested by Bartschat \textit{et al} [9] who implemented an explicit numerical Schmidt orthogonalization procedure. It has been shown that the standard low-energy $R$-matrix codes (RMATRIX II), when amended to allow for a large number of pseudo-states, can yield very accurate results at both low and intermediate energies for electron scattering from atomic hydrogen. The importance of this development lies in the fact that the same computer codes can be used to study electron scattering by many-electron targets. This opens the door to scattering calculations involving complex atoms and ions at intermediate energies. Later, Badnell and Gorczyca [10] introduced an alternative approach, namely diagonalization of the overlap matrix between the two orthogonal bases. They incorporated Laguerre pseudo-states in the more general RMATRIX I code, which allows for relativistic effects and can describe photoionization. This code and later its parallelized modifications were widely used for different targets, albeit concentrating again on quasi-one or quasi-two electron targets [11]. The application of this code to complex atoms such as Ne [12] or Ar [12] is still somewhat restricted, with convergence not always being achieved.

The basic idea in different implementations of the RMPS method is always the same: the target Hamiltonian is diagonalized in a basis of finite range, whether it be a box with a hard wall like the $R$-matrix radius or a soft wall as in a Laguerre or Sturmian basis. States whose orbitals effectively fit in the box are excellent approximations of the physical target states. Then there will be some states whose physical orbitals do not quite fit but whose energies are still below the ionization threshold, and then there are states above that threshold. The former set approximate the effect of the high-lying Rydberg states while the latter simulate the ionization continuum. We use the box-based method, which perfectly matches our using $B$-splines as an universal basis for both bound and scattering orbitals. Below we illustrate our approach with the example of new calculations for the e-Ar problem.

The target states were generated by combining the multiconfiguration Hartree-Fock (MCHF) and the $B$-spline box-based close-coupling methods. Specifically, the structure of the multichannel target expansion in intermediate–coupling scheme was chosen as
\[
\Phi(3s^23p^5nl,J) = A \sum_{n,l,s} \{\varphi(3s^23p^5;\frac{1}{2},J) \cdot P(nl),LS\}^j + A \sum_{n,l,s} \{\varphi(3s3p^6;\frac{1}{2},S) \cdot P(nl),LS\}^j + a\phi(3s^23p^n)S_0
\]

where \(P(nl)\) denotes the orbital of the outer valence electron, while the \(\varphi\) and \(\phi\) functions represent the configuration interaction (CI) expansions of the corresponding ionic or specific atomic states, respectively. The expansion (1) can be considered as a model for the entire \(3s^23p^5nl\) and \(3s3p^6nl\) Rydberg series in Ar, including the continuum pseudostates lying above the ionization limit. Although this expansion can also provide a good approximation for the ground state, we chose to use a separate CI expansion for this state by directly including relaxation effects via state-specific one-electron orbitals. This illustrates the additional flexibility of our code for a more accurate description of individual states if needed. Inner-core (short-range) correlation is accounted for through the separately optimized CI expansions for the ionic states.

The unknown functions \(P(nl)\) for the outer valence electron were expanded in a \(B\)-spline basis. The \(B\)-spline coefficients, along with the coefficient \(a\) for the ground state, were obtained by diagonalizing the atomic Hamiltonian in the Breit-Pauli approximation, with the condition that all orbitals vanish at the boundary. Since the \(B\)-spline bound-state close-coupling calculations generate different nonorthogonal sets of orbitals for each atomic state, their subsequent use is somewhat complicated in comparison to standard application of \(R\)-matrix codes with orthogonal set of orbitals.

The scattering calculations were carried out with a newly developed, fully parallelized version of the BSR complex. The \(R\)-matrix radius was set to 25 \(a_0\), where \(a_0 = 0.529 \times 10^{-10}\) m is the Bohr radius. We employed 65 \(B\)-splines to span this radial range using a semi-exponential grid of knots, with the maximum interval in this grid chosen as 0.6 \(a_0\). This is sufficient to treat electron scattering up to 300 eV. Our close-coupling expansion includes 500 states of argon, with the lowest 78 states representing the bound spectrum and the remaining 422 the target continuum. We included all \(3s^23p^5nl\) and \(3s3p^6nl\) states with \(l = 0–3\). This model will be referred to as BSR-500 below. The continuum pseudostates cover the energy region up to 45 eV. The above scattering model contained up to 2460 scattering channels. For a given \(B\)-spline basis, this number defines the size of the matrices involved and leads to generalized eigenvalue problems with matrix dimensions up to 150 000. Matrices of such dimensions can be handled with our current computational resources presented at the Texas Advanced Computing Centre (http://www.tacc.utexas.edu/).

The angle-integrated cross sections (ICSs) for excitation of the two \(3p^54s\) states are presented in figure 1. We compare our new results with those from the 31-state \(B\)-spline \(R\)-matrix calculation (BSR-31) [14], with available experimental data [15,16,17]. We see significant difference between the present results and our previous BSR-31 calculations, which include only the bound states of argon. The pseudostates not only further reduce the predicted cross sections but also change their energy dependence. The discrete-state-only \(R\)-matrix cross sections rise rapidly just above the ionization limit, while the results obtained with the pseudostates included do not. Although the most significant effects of continuum coupling occur above the ionization limit, they persist down into the bound-state energy region.

A more detailed study of the convergence of the close-coupling expansions is presented in the bottom panels of figure 1. The BSR-5 model contains only the four \(3p^54s\) states, and hence their results are expected to be close to what one might obtain in a distorted-wave approximation with the same target description. The differences between the BSR-5 and BSR-31 results illustrate the effects of coupling to the higher-lying bound states. This coupling considerably reduces the theoretical cross sections near the maximum and is responsible for the resonance structure at low energies. The entire influence of discrete-state excitation is represented by the BSR-78 model, containing all bound states of argon obtained with the given box radius. The BSR-160 model contains additionally from 4 to 10 continuum pseudostates \(3p^5kl\) for each angular symmetry (or two pseudostates for each \(kl\)), covering the region up to 2 eV above the ionization threshold. As seen from figure 1, these low-lying continuum pseudostates have a strong influence on the 4s cross sections, especially for excitation of
the metastable state, leading to additional structure in the energy dependence around 20 eV. The influence of the continuum pseudostates is gradually reduced with increasing projectile energy, and all scattering models converge to each other around 200 eV where the coupling effects are expected to be small. This is about ten times the ionization energy. Our most extensive calculations, BSR-600, show very similar results as the BSR-500 model, indicating that we reached convergence at all energies.

Figure 1. Angle-ICSs for the electron-impact excitation of the 3p⁵4s states in argon.

The agreement between the present results and various experimental data is rather scattered. All experimental ICS were obtained from differential cross sections (DCSs) measurements at fixed energies in crossed-beam setups. These DCSs were extrapolated to 0° and 180° and then integrated to yield absolute excitation cross sections as a function of incident electron energy. Uncertainties in this method necessarily arise from the unknown behavior of the DCS at small and large scattering angles, especially if somewhat questionable theoretical predictions are used as a guide. These uncertainties are almost certainly responsible for the scatter in the energy dependence of the experimental ICSs.

As seen from figure 1, coupling to the continuum is equally important for both the weak "exchange" transition to the (3p⁵4s)³P₂ level and for the strong dipole-allowed transition to the (3p⁵4s)³P₁ level, and its influence persists over a wide range of electron energies. The new BSR-500 results are lower than the BSR-31 cross sections by 20-40% at intermediate energies from 30 eV to 150 eV. We obtain the closest agreement with the early measurements of Chutjian and Cartwright [17]. New absolute measurements are highly desirable. The strong influence on the dipole transition was originally unexpected, but it was found for many other transitions, including the excitation of the (3p⁵3d)³P level where the corrections reach factors up to 10.

3. Ionization

We consider the ionization of an atom by electron impact, schematically written as

\[ e_0(k_0, \mu_0) + A(L_\alpha S_\alpha) \rightarrow e_i(k_i, \mu_i) + e_e(k_e, \mu_e) + A^+(L_f S_f) \]  \hspace{1cm} (2)

where \( k_i \) and \( \mu_i \) (\( i=0,1,2 \)) are the linear momenta and spin components of the incident, scattered, and ejected electrons, respectively. \( L_\alpha, S_\alpha \) and \( L_\gamma, S_\gamma \) are the orbital and spin angular momenta of the initial \((N+1)\)-electron atom and the residual \( N \)-electron ion. For a complete description of this process, we need the ionization amplitude

\[ f(L_\alpha M_\alpha S_\alpha M_{\gamma \alpha}, k_0, \mu_0 \rightarrow L_f M_f S_f M_{\gamma f}, k_i, \mu_i k_e, \mu_e) , \]  \hspace{1cm} (3)
where we have introduced the magnetic quantum numbers of the atomic ($M_0$) and ionic ($M_j$) orbital angular momenta, as well as the corresponding spin components $M_{S_j}$ and $M_{S_f}$.

In our BSR pseudostate approach [4], we proceed as follows. For a given energy of the incident electron, we obtain the scattering amplitudes $f^p(L_0M_{0j}S_0M_{S_j},k_0\mu_0 \rightarrow LMSM_{j},k_1\mu_1,k_2\mu_2)$ for excitation of all atomic pseudostates $\Phi^p(L_p,S_p)$. We then obtain the ionization amplitude (2) by projecting the excitation amplitudes to the true continuum functions $\Psi^{k,j,(-)}_{L,M,S,M_{S_j}}$, and summing over all energetically accessible pseudostates using the ansatz

$$f(L_0M_{0j}S_0M_{S_j},k_0\mu_0 \rightarrow L_fM_{fj}S_{fj},k_1\mu_1,k_2\mu_2) = \sum_p \psi^{k,j,(-)}_{L,M,S,M_{S_j}} |\Phi^p(L_p,S_p)| f^p(L_0M_{0j}S_0M_{S_j},k_0\mu_0 \rightarrow LMSM_{j},k_1\mu_1,k_2\mu_2)$$

(4)

This requires the determination of the overlap factors $<\psi^{k,j,(-)}_{L,M,S,M_{S_j}} |\Phi^p(L_p,S_p)>$ between the true continuum states and the corresponding pseudo-states. The continuum states $\Psi^{k,j,(-)}_{L,M,S,M_{S_j}}$ are obtained using the R-matrix method with the same close-coupling expansion that is employed for the pseudostates (see (1) as example). Computationally, the only difference is the use of R-matrix boundary conditions by adding the corresponding Bloch operator. Note that the one-electron pseudo-orbitals and the continuum orbitals are not orthogonal. Our nonorthogonal orbital technique takes this nonorthogonality into account to full extent for any many-electron atom. It is, however, worth pointing out an important subtlety of the approach. Note that $\Psi^{j}_f$ and $\Phi^p$ have different energies for the continuum electron represented by $k_f$ and the electron in the pseudo-state. Having noted numerical instabilities in some cases, Bray et al [18] suggested interpolating the transition-matrix elements as an alternative. While this interpolation, indeed, worked very well for the single-channel case, our direct projection method is necessary to maintain the crucial channel information in multi-channel situations that will be illustrated below. Finally, the triple-DCS for ionization with the residual ion remaining in the final state $f$ (this may include simultaneous ionization-excitation) is given by

$$\frac{d\sigma_f}{d\Omega dS_d dE} = \frac{k_f}{k_0} \frac{1}{2(2L_0 + 1)(2S_0 + 1)} \sum_{m_f,m_{S_f}} \sum_{m_{S_j}} f(L_0M_{0j}S_0M_{S_j},k_0\mu_0 \rightarrow L_fM_{fj}S_{fj},k_1\mu_1,k_2\mu_2)$$

(5)

Another issue worth mentioning in this context is the size of the R-matrix box. In order to span a large energy range with relatively few basis functions, the box was made as small as possible. For ionization, however, the size of the box and the related range of the pseudo-states determine the region where correlation effects between the two outgoing electrons are still properly accounted for. Consequently, one often uses a much larger box than needed to simply ignore exchange between the projectile and the bound target electrons.

The validity of the above approach was first tested for electron-impact ionization of helium in its ground state, leaving the residual He$^+$ ion also in its ground state [4,19]. This process has been widely studied in the literature, and numerous experimental benchmark data and predictions from other methods are available for comparison. Our scattering model contained 525 coupled states with $S,P,D$, and $F$ symmetry. The energetically lowest 11 states describe the physical bound states of He up to principal quantum number $n = 3$, while the rest are pseudostates that approximate the Rydberg spectrum (ten states) and the ionization continuum up to 100 eV (479 states). We obtained overall very close agreement with results from other nonperturbative approaches, convergent close coupling (CCC) and time-dependent close coupling (TDCC), for a variety of kinematical situations, including single-, double- and triple-differential cross sections, as well as for the total cross section for energies up to 300 eV. In particular, we confirm the 10-15% reduction in the total cross section due to correlation effects in the ground state, which drops the theoretical prediction in agreement with the more recent experimental data.
Figure 2. TDCS ratio for the electron-impact ionization of He(1s^2) leaving the residual ion in either the He^+(1s) or the He^+(n = 2) states.

Figure 3. Absolute cross sections for simultaneous electron-impact ionization of excitation of He(1s^2) leaving the residual ion as He^+(2p).

The most significant progress achieved by the BSR with pseudostates method was the first-time successful description of a much more complex process, namely the ionization of one 1s electron and simultaneous excitation of the other one. This is a highly correlated four-body Coulomb process that posed major problems to theoretical attempts for many years. Figure 2 compares the BSR predictions with the directly measured experimental cross section ratios [19] for ionization without excitation (leaving the electron in He^+ in the 1s state) and ionization with excitation to He^+(2s + 2p). The agreement with the experimental data is excellent at all angles of the reference electron between 24° and 56°, and all detection angles of the other electron between 25° and 115°.

There is also a long-standing controversy regarding the absolute value of the total cross section for simultaneous ionization plus excitation of helium in the He^+(2p), presented in figure 3. The last measurements by Merabet et al [22] suggested three-times lower cross sections in comparison to earlier absolute normalizations [23]. Available theoretical results [25] are scattered and cannot resolve the problem. Our BSR results clearly favor the earlier normalization [23]. Taking into account the close agreement BSR results for both total ionization cross section and the (n=1)/(n=2) ratios discussed above, the absolute normalization for the ionization plus 2p-excitation cross sections can be considered as finally established.

The study of more complex targets (e.g., neon, argon, etc) impose additional problems in the description of the target structure. Until very recently, most theoretical work on such targets was still based on variants of the distorted-wave Born approximation (DWBA) [28] and the first-order (DWB1-RM) or second-order (DWB2-RM) hybrid distorted-wave + R-matrix approach [29]. Despite some success, problems for the low-energy regime prevailed due to a less than ideal (if any) description of the PCI between the two outgoing electrons. The present BSR with pseudostates approach overcomes these problems by using a more correlated description of the entire scattering system.

Figure 4. Three-dimensional triple-differential cross section for 2p ionization of neon.
Very recently, an experiment was performed for Ne(2p) the ionization at an incident electron energy of 100 eV \[5\], with particular emphasis on proper cross-normalization of the results. The experiment was carried out by employing an advanced reaction microscope, allowing to measure full three-dimensional differential cross sections (3DCS). Since the entire experimentally accessible phase space is measured simultaneously, all relative 3DCS are cross-normalized, and only a single global factor is required to compare theory and experiment. This factor puts the 3DCS on an absolute scale.

Examples for three-dimensional 3DCS patterns for a projectile scattering angle of 10° are presented in figure 4. The left panels represent the measured data while the BSR prediction is shown on the right. In this particular representation, the relative 3DCS is given by the radial distance from the origin to the surface of the plot. The projectile with momentum \( p_o \) enters the interaction region from below and after scattering has the momentum \( p_e \). The momentum transfer to the target system is indicated by the arrow labeled \( q \). Two general features are observable. Electrons emitted roughly in the direction of the momentum transfer form the binary peak, while those emitted in the opposite direction form the recoil peak. Due to the low energy of the projectile, PCI is strong (as expected) and, consequently, the binary peak is suppressed near the forward direction.

The qualitative comparison of experiment and theory shows very good overall agreement, with the suppression of the binary peak towards the forward direction being slightly more pronounced in the experimental data. The global scaling factor used to normalize the experimental data to the BSR theory was found by achieving the best fit to the binary peak in the scattering plane. It was subsequently applied to all other (48 total) kinematics and planes, with overall impressive agreement between experiment and the BSR predictions, not only with regard to the angular dependence for each fixed set of final-state electron energies and detection angle of the projectile, but also the cross-normalization.

![Graph](image)

**Figure 5.** Total cross sections for electron scattering from neon and argon.

4. Generation of extensive datasets for plasma modelling

Finally, we close the circle by showing how the detailed results above can be useful for applications. Figure 5 compares the total (elastic + excitation + ionization) cross section for electron collisions with Ne and Ar atoms in their ground state with a number of experimental data. Our BSR calculations were able to reproduce the cross sections in a single calculation for energies between 0.01 eV and 200 eV. The figure also shows the relative importance of the contributions from individual collision processes. Elastic scattering dominates over the entire energy regime shown in the figure. We note the accurate description of the Ramsauer-Townsend minimum in Ar, which is very sensitive to the ground-state polarization included. Excitation processes provide a relatively small contribution to the total cross section, while ionization becomes more and more important with increasing projectile energy. The overall excellent agreement with the available experimental data confirms the accuracy of the present approach. These results, including the important momentum-transfer cross sections, are now available through the publicly accessible LXCAT database (www.lxcat.net).
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