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# The $B$-spline $R$-matrix method in low-energy electron scattering on complex atoms

**E.A. Nagy, S.V. Gedeon, V.F. Gedeon, V.Yu. Lazur**

*Department of Theoretical Physics, Uzhhorod National University, 53 Voloshina, 88000 Uzhhorod, Ukraine*

**Abstract**

This paper provides an overview of the systematic application of the $B$-splines $R$-matrix method (BSR) to calculate of electron-atom collision processes. This method allow to use the term-dependent nonorthogonal orbitals along with $B$-splines as basis functions. Thus, it provides the effective accounting of electron correlation. The cases of the slow electrons scattering on the Ca, Mg, Sr, Si, F, Al, and B atoms have been considered. The obtained calculations results are in good agreement with a large set of experimental data in a wide range of collision energies.

## 1 Introduction

Over the past decade, the physics of electron-atom (EA) collisions has been developed quite intensely. This is caused by both fundamental nature of the investigated processes and application needs. The elementary processes of electron-atom interaction, that accompanying such collisions, are extremely diverse. Therefore, the main problem is the deep-level understanding of the behavior of submicroscopic and often strongly correlated quantummechanical many-body systems. This knowledge allows to obtain a large massive of data needed to simulate the behavior of various types of plasmas and discharges, and to evaluate their properties. It concerns, firstly, the characteristics of the atomic structure; secondly, cross-sections and collision velocities of electrons and photons collisions with atoms and ions. A considerable number of common computer programs have been developed for these purposes (see., eg, [1]). Using these program codes the numerical calculations of EA-scattering characteristics with rapidly increasing complexity were performed. Comparison with experimental data shows the reliability of computer programs used in these calculations. This is especially important when the theory is the only source of the systematic data sets.

This article is devoted to the $B$-spline $R$-matrix method (BSR) [2]. Extensive information about usage of this approach is given in [1]. However, many aspects of the the BSR-method application still are not closed. In this paper, we will focus on the most important points of BSR-calculations of electron processes with

Ca [3, 4], Mg [5], Sr [6], Si [7], F [8], B [9], and Al [10] atoms, that were performed by our research group.

## 2 The research method

BSR method [2] is quite versatile. It has been successfully applied for the structural calculations of atomic systems, and for the interpretation of the processes of elastic and inelastic electron-atom collisions. It is desirable to calculate all of these processes within the framework of the same comprehensive approach. Appropriate clarification made using boundary conditions for the close coupling (CC) equations. In addition the different physical effects are taken into account: the electronic correlations, threshold phenomena, channels coupling. Although the BSR method can be applied to heavy atoms, we will work here exclusively with the light atomic targets.

Note that most of the available theoretical methods can work only with relatively simple quasi-one-electronic (hydrogen-like) and quasi-two-electronic (helium-like) targets. In contrast, BSR method allows consideration of the complex targets with open shells. The $B$-spline $R$-matrix method [2], that we used in the calculations [3]-[10], is different from the other approximations by the presence of two innovations. First one is the usage of non-orthogonal orbitals for representation of radial parts of one-electron wave functions. This applies both to the bound atomic states, and to the states of the scattered electron. Second one is the usage of felicitous $R$-matrix basis, which is defined by a full finite set of the $B$-splines with compact carriers in the inner region.

So, in [2] the standard methods of close coupling of channels and $R$-matrix (see.Burke [11]) were in fact generalized for the case of low-energy electron interaction with arbitrary complex atom. In the CC-approximation the problem of low-energy electron scattering on the $N$-electron atom is reduced to the solution of the Schrödinger equation

$$(H_{N+1} - E)\,\Psi_\alpha^\Gamma(X, x_{N+1}) = 0, H_{N+1} = \sum_{i=1}^{N+1}\left(-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right) + \sum_{i>j=1}^{N+1}\frac{1}{r_{ij}} \qquad (1)$$

with appropriate boundary conditions. Here $E$ and $H_{N+1}$ are the total energy and the Hamiltonian of the $(N+1)$-electron system „target atom + projectile electron", $Z$ is nuclear charge. The Hamiltonian $H_{N+1}$ (1) is diagonal with respect to the total orbital angular momentum $L$, the total spin $S$, their projections $M_L$, $M_S$ on a given axis and parity $\pi$. The function $\Psi_\alpha^\Gamma(X, x_{N+1})$, which is usually called „the collision wavefunction", is a fully antisymmetrized wavefunction of the $(N+1)$-electron system; $X \equiv (x_1, ..., x_N)$ and $x_i \equiv (\vec{r}_i, \sigma_i)$ refers to the set of spatial $\vec{r}_i$ and spin $\sigma_i$ coordinates of the $i$th electron. Furthermore, $\Gamma \equiv (\gamma L S M_L M_S \pi)$ is a complete set of quantum numbers of the $(N+1)$-electron system. The subscript $\alpha$ characterizes the initial conditions and usually denotes the incoming scattering channel. Without ionization the expansion of the total collision wavefunction

$\Psi_\alpha^\Gamma(X, x_{N+1})$ can be written as

$$\Psi_\alpha^\Gamma(X, x_{N+1}) = A\sum_{i=1}^{n} \overline{\Phi}_i^\Gamma(X; \widehat{r}_{N+1}, \sigma_{N+1}) \frac{F_{i\alpha}^\Gamma(r_{N+1})}{r_{N+1}} + \sum_{j=1}^{m} c_j \chi_j^\Gamma(X, x_{N+1}). \quad (2)$$

The index $i$ includes all quantum states of the system, and $\overline{\Phi}_i^\Gamma$ is a channel function that is obtained by vector coupling of $N$-electron target wavefunction $\Phi_i(X) \equiv \Phi_i(x_1, ..., x_N)$ with angle $Y_{l_T m_T}(\widehat{r}_{N+1})$ and spin $\chi_{m_S}^{1/2}(\sigma_{N+1})$ parts of wavefunction $(N+1)$th scattered electron. In the formula (2) $A$ - is the antisymmetrization operator with respect to the exchange of any pair of electrons, while $F_{i\alpha}^\Gamma(r_{N+1})$ is the radial component of the scattered electron wavefunction when the target is in the $i$th state. The $\chi_j^\Gamma(X, x_{N+1})$ is a set of square integrable antisymmetric correlation functions. Together with $\Phi_i(X)$, they considered known. The challenge is to find the radial functions of scattered electron $F_{i\alpha}^\Gamma(r_{N+1})$ and the expansion coefficients $c_j$. In the case of complex atoms the wave functions $\Phi_i(X)$ are constructed in the form of multiconfiguration expansion

$$\Phi_i(x_1, ..., x_N) = \sum_j c_{ij} \varphi_j(x_1, ..., x_N), \quad (3)$$

where the known configurations $\varphi_j$ are constructed from a one-electron bound orbital basis, usually consisting of physical self-consistent field orbitals plus possibly additional pseudo-orbitals. The latter are included to represent correlation effects. The coefficients $c_{ij}$ in (3) are determined by diagonalizing of the $N$-electron target Hamiltonian:

$$\langle \Phi_i | H_N | \Phi_j \rangle = E_i(Z, N) \delta_{ij}. \quad (4)$$

Typically, the first sum in the right part of the expansion (2) include only the state of the target, which at given energy $E = E_i + k_i^2/2$ correspond to so-called open channels. In the first sum can also be included some pseudo-states. They are approximate states of the continuous spectrum. Selection of the pseudo-state is carried out on the basis of an accurate accounting of the polarizability of the ground and several excited states of the target. In addition to using the pseudo-states, the contributions of selected channels can be partially taken into account through accounting a finite number of correlation functions $\chi_j^\Gamma(X, x_{N+1})$, included in the second sum of expansion (2).

The basis functions $\varphi_j$ and $\chi_j$ in expansions (2), (3) are constructed of the single-electron atomic orbitals $\varphi_{\alpha_i}$, that in the central field approximation have the form

$$\varphi_{\alpha_i}(x) = 1/r \cdot P_{n_i l_i}(r) Y_{l_i m_i}(\widehat{r}) \chi(m_S|\sigma), x \equiv (\vec{r}, \sigma) \quad (5)$$

where $\alpha_i$ – is a short designation for a set of quantum numbers $n_i$, $l_i$, $m_i$ and $m_S$. In the standard approach (see Burke [11]) for the convenience of computing, the radial wave functions of the scattered electrons $F_{i\alpha}^\Gamma$ are chosen orthogonal to all atomic orbitals $P_{n_j l_j}$ of the same target symmetry, that is,

$$\int_0^\infty P_{n_j l_j}(r) F_{i\alpha}^\Gamma(r) dr = 0, \quad l_j = l_i. \quad (6)$$

It is clear that this condition is purely mathematical, and not a physical requirement. This condition does not follow from the general quantum-mechanical principles, because the radial orbitals $P_{n_j l_j}$ and $F^{\Gamma}_{i\alpha}$ are eigenfunctions of different Hamiltonians. Condition (6) actually means, that the incident electron can not be virtually trapped in one of the unoccupied subshells, that are accounted in the target states expansion (3). In the standard approach framework [11] the possibility of such capture is provided by inclusion in second sum of expansion (2) of the special additional correlation functions $\chi^{\Gamma}_j$. This leads to a non-physical pseudo-resonant structures in cross sections. It also causes a significant increase the number of integral-differential equations, that must be are solved. In our studies [3]-[10] it has been shown that these difficulties can be eliminated. It is enough to waive the requirement of orthogonality (6) functions $F^{\Gamma}_{i\alpha}$ to target orbitals $P_{n_j l_j}$. This allows to take into account the possibility of a virtual capture of an electron into unfilled subshell of the target.

Let's substitute the expansion (2) into the equation (1) and sequentially multiply on the functions $\overline{\Phi}^{\Gamma}_i$ and $\chi^{\Gamma}_j$. After integration in all the variables, except $r_{N+1}$, we obtain a system of integral-differential equations for the functions $F_i \equiv F^{\Gamma}_{i\alpha}$:

$$\Big(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l_i(l_i+1)}{r^2} + \frac{2Z}{r} + k_i^2\Big)F_i(r) = 2\sum_j \Big(V_{ij} + W_{ij} + X_{ij}\Big)F_j(r), \qquad (7)$$

where $k_i^2 = 2\,[E - E_i(Z,N)]$, and $V_{ij}$, $W_{ij}$, $X_{ij}$ – is the local direct, non-local and non-local exchange correlation potentials, respectively. In the case of EA-scattering the explicit form of these potentials is automatically generated by BSR program [2].

In our studies [3]-[10] to solve the system of CC-equations (7) was applied the $B$-splines $R$-matrix method. It is based on the use of non-orthogonal orbitals. As the basis functions are used $B$-splines. $R$-matrix method implies the split of the configuration space of the system „atom + electron" into two areas: the inner $r < a$ and external $r > a$. The radius of the inner region of $r = a$ is chosen so that the exchange and correlation effects were quite small for $r \geq a$. Full wavefunction of $(N+1)$-electron system in the inner region at a given energy $E$ is given by expansion

$$\Psi^{\Gamma}_E = \sum_k A^{\Gamma}_{Ek}\Psi^{\Gamma}_k, \qquad (8)$$

where $\Psi^{\Gamma}_k$ – is the energy-independent discrete basis set:

$$\begin{aligned}\Psi^{\Gamma}_k(X, x_{N+1}) &= A\sum_{i,j}\bar{\Phi}^{\Gamma}_i(X;\hat{\mathbf{r}}_{N+1},\sigma_{N+1})\frac{u_j(r_{N+1})}{r_{N+1}}c^{\Gamma}_{ijk} + \\ &+ \sum_i \chi^{\Gamma}_i(X, x_{N+1})d^{\Gamma}_{ik}. \qquad (9)\end{aligned}$$

Here $\overline{\Phi}^{\Gamma}_i$ and $\chi^{\Gamma}_i$ are defined the same way as in the formula (2). Function $F^{\Gamma}_{i\alpha}$ describe the radial movement of the scattered electron in the $i$-th channel. We have presented them in the form of a linear combination of a finite number of basis

functions $u_j$, which satisfy boundary conditions: $u_j = 0$, $(a/u_j)du_j/dr|_{r=a} = b$, where $b$ is an arbitrary real constant. For such basis functions, the Hamiltonian (1) is not a Hermitian in the inner region. This is a consequence of non-zero values (at $r = a$) surface terms arising from the kinetic energy operator. However, these members can be removed using the Bloch operator $L_{N+1}$ [11]. The formal solution of Schrodinger equation (1) acquires the form of

$$|\Psi\rangle = 1/2 \sum_{kj} |\Psi_k^\Gamma\rangle\langle\Psi_k^\Gamma|\bar{\Phi}_j\rangle(E_k - E)^{-1}(d/dr_{N+1} - b_j/r_{N+1})\langle\bar{\Phi}_j^\Gamma|\Psi\rangle. \qquad (10)$$

Projecting this equation onto the channel function $\overline{\Phi}_i^\Gamma$ and performing calculations on the border of the inner region, we obtain

$$F_i^\Gamma(a) = \sum_{j=1}^{n} R_{ij}^\Gamma(E)\left(a\frac{\mathrm{d}F_j^\Gamma}{\mathrm{d}r_{N+1}} - b_j F_j^\Gamma\right)_{r_{N+1}=a}, \qquad (11)$$

where we have introduced the $R$-matrix with elements

$$R_{ij}^\Gamma(E) = \frac{1}{2a}\sum_k \frac{\omega_{ik}^\Gamma(a)\omega_{jk}^\Gamma(a)}{E_k^\Gamma - E}, \qquad (12)$$

the reduced radial wavefunctions $F_i^\Gamma$ and the surface amplitudes $w_{ik}^\Gamma$. Diagonalizing a matrix $\langle\Psi_k^\Gamma|H_{N+1} + L_{N+1}|\Psi_{k'}^\Gamma\rangle_{\mathrm{int}}$ for each set of quantum numbers of $\Gamma$, it is possible to determine the energy $E_k^\Gamma$ and coefficients $c_{ijk}^\Gamma$, $d_{ik}^\Gamma$ in the expansion (9), i.e. find the wave functions $\Psi_k^\Gamma$ for the respective basic states. However, it should be done only once, to determine the $R$-matrix over the entire range of collision energies.

By inclusion in the expansion (9) of the additional correlation functions $\chi_i^\Gamma$ one can partially take into account the effects related to the orthogonality conditions (6) for functions $F_{i\alpha}^\Gamma$ and with limitation of the first sum in (9) by a finite number of terms. However, in most cases this leads to the appearance of a pseudo-resonant structure in the cross sections. In addition, it excessively increases the number of additional integral-differential equations. These equations must be left in (9) to provide a realistic calculation of the complex atoms and the processes of their interactions with electrons.

As noted above, the proposed in [2] BSR method is free from these difficulties. It is based on the use of nonorthogonal orbitals to represent the one-electron wavefunctions for both discrete and continuous spectra. Another key aspect of the BSR-version of the $R$-matrix method is the choice of $B$-splines as basis functions $u_j(r)$ in the $R$-matrix representation (9) for the inner region. This choice $u_j(r)$ provides fast convergence $R$-matrix decomposition without including in the diagonal $R$-matrix elements (12) of any Buttle corrections. $B$-splines have the properties as if specially created for the $R$-matrix theory.

They constitute a complete basis on the finite $R$-matrix interval $[0, a]$ and are convenient for finding both the bound target orbitals and the orbitals of the scattered electron. Convenience primarily consist in the fact that $B$-splines are the finite functions and have non-zero values on the carrier-intervals only.

The solution of CC-equations (9) in the outer region $r > a$ and the crosslinking of solutions at the boundary $r = a$ allows to determine the $K$- and $S$-matrix, and the phase shifts. In the outer area all exchange and correlation potentials are practically zero. Therefore, in this area we get a fairly simple system of coupled integral-differential equations for radial functions $F_i(r)$. It can be accurately solved numerically using modern computers. These solutions are sewn at $r = a$ with the solutions from the internal region $r < a$. After this it is easy to determine the $K$-matrix from the asymptotic relation

$$F_{i\alpha} \underset{r\to\infty}{\sim} k_i^{-1/2}(\sin(\theta_i)\delta_{i\alpha} + \cos(\theta_i)K_{i\alpha}). \tag{13}$$

Here, the second index $\alpha$ indicates the channel number of the incident wave. Scattering matrix $S_{i\alpha}$ and transition matrix $T_{i\alpha}$ with $n \times n$ dimensions are determined by known matrix relations $\mathbf{S} = \mathbf{1} + \mathbf{T} = (\mathbf{1} + i\mathbf{K})/(\mathbf{1} - i\mathbf{K})$. These matrices are then used to calculate the scattering cross sections and all other observable values.

The most important from a computational perspective properties of $B$-splines are described in [2] (and the references therein). There's also discussed in detail spline algorithms for solving differential and integro-differential equations and the bound states scattering problem. In particular, there were demonstrated their fundamental advantages over the algorithms based on the finite-difference approximation.

In the BSR approximation [2] is used a common approach to the problem of accounting the correlation of electrons, often with the use of the results of a multiconfiguration Hartree-Fock method (MCHF) [12, 13]. It is based on the representation of radial orbitals $P_{nl}(r)$ in the form of a finite expansion on a complete basis set of $B$-splines $\{B_i\}_{i=1}^{n_S}$. Multi-configurational character of expansion (3) for total wavefunction of $N$-electronic system, allows you to take into account a significant part of the correlation effects. Quantum-mechanical calculation within MCHF method consists of two phases: constructing the many-electron CSF-basis and solving the multiconfiguration Hartree-Fock equations.

From these equations, are determined the radial wave-functions $P_{nl}(r)$, which are part of Slater determinants. Calculation results of the atomic characteristics are highly dependent on the choice of radial orbitals $P_{nl}(r)$ and configurations that are included in the expansion of the target wavefunction. At the same time the term-dependent non-orthogonal bound orbitals are used as one-electron functions. They are optimized in the independent calculations for individual terms. The use of such orbitals allows a detailed description of the resonant structure in the low-energy EA-scattering cross sections.

Note that the calculations for the external region was performed using the flexible asymptotic $R$-matrix (FARM) package [14].

# 3 Results and discussion

In [3] has been investigated the low-energy electron scattering from Ca atoms and photodetachment of $Ca^-$. The low-energy range from threshold to 4 eV was explored. The multiconfiguration Hartree-Fock method with nonorthogonal orbital sets was used for an accurate representation of the target wave functions.

The close-coupling expansion includes 39 bound states of neutral calcium, covering all states from the ground state to $4s8s\ ^1S$. The BSR-calculations [3] yield good agreement with the few available experimental data for both elastic electron scattering and photodetachment of $Ca^-$. The prominent resonance structure in the low-energy region was analyzed and discussed.

In the continuation of studies [3], in the paper [4] the $B$-spline $R$-matrix (close-coupling) method was applied to study electron impact excitation of the four lowest excited states of calcium. Results for angle-integrated and angle-differential cross sections, as well as (pseudo-) Stokes parameters of the light emitted in the $4s4p\ ^1P_0 \to 4s^2\ ^1S$ optical decay, were compared with various experimental data and predictions from other close-coupling and distorted-wave calculations. Overall, the agreement between our results and the experimental data is very satisfactory, although a few discrepancies remain.

In paper [5] $B$-spline $R$-matrix (close-coupling) method was used to perform a systematic study of angledifferential and angleintegral cross sections for electron scattering from neutral magnesium. The calculations cover elastic scattering and excitation of the five excited states $3s3p\ ^{1,3}P^o$, $3s3d\ ^1D$, $3s4s\ ^1S$ and $3s4p\ ^1P^o$. A multiconfiguration Hartree-Fock method with nonorthogonal orbitals was applied for an accurate representation of the target wave functions. The close-coupling expansion for the collision problem included 37 bound states of neutral magnesium. Angle-differential cross sections are presented for incident electron energies from 10 to 100 eV. The calculation results have appeared very sensitive to the effects of electron correlations in Mg target, as well as in the $(N+1)$-electron system $e-$Mg scattering. The use of the term-dependent non-orthogonal sets of orbitals $P_{n_j l_j}$ and $F^{\Gamma}_{i\alpha}$ allowed to describe accurately both the scattering states and the target states of Mg atom. The valence and core-valence correlations were taken into account by including in the multiconfiguration expansion of the wavefunctions the target electron configurations with an excited core. Calculation results for elastic scattering DCS (Fig. 1) at 10, 15, 20, 40, 60, 80, and 100 eV, as well as the corresponding angle-integrated cross sections, were compared with various experimental data and predictions from other close-coupling and distorted-wave calculations. In spite of a few remaining discrepancies, the overall agreement between our results and the experimental data is very satisfactory.

Consider the electronic excitation of the optically allowed transition $3s^2\ ^1S^o \to 3s3p\ ^1P^o$. The calculated angular dependences of DCS are in good agreement with the results of recent measurements [18] at energies of 10, 15, 20 and 40 eV. They are characterized by the appreciable angular asymmetry with predominant scattering in the region of small angles. For excitation of the spin-forbidden transition $3s^2\ ^1S^o \to 3s3p\ ^3P^o$ both the experimental, as well as theoretical data are somewhat contradictory. The cross sections of this transition is very sensitive both to minor refinements of the target wavefunctions, as well as to the effects of coupling of channels, including the coupling with the ionization continuum. The results of BSR37-calculations of the DCS [5] for the electron excitation of three more $3s4s\ ^1S$, $3s3d\ ^1D$ and $3s4p\ ^1P^o$ states of Mg atoms also are in good agreement with the experimental data [19]. This further confirms the accuracy of the BSR approximation.

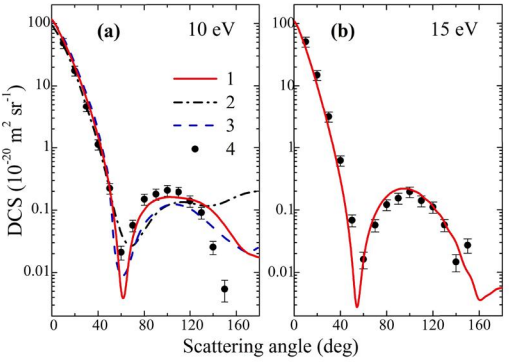


Figure 1: Angle-differential cross sections for elastic $e$-Mg scattering at impact energies of 10, and 15 eV: 1 – our BSR37-calculation [5]; 2 – CC5 [16]; 3 – a method of optically coupled channels [17]; 4 – experiment [15]

In paper [6] were studied the slow electron scattering processes on strontium atoms. In this work were numerically calculated excitation energies of the 31 lower states of the Sr atom. The calculations were performed using MCHF method with term-dependent nonorthogonal orbitals $P_{nl}(r)$. We have obtained excitation energies which are in good agreement with the experimental values. Electron correlations were taken into account by including in MCHF-expansion basis the functions with singly and doubly excited electron configurations. In the BSR31-approximation there were calculated the energy and angular dependencies of DCS and ICS for the elastic and inelastic electron scattering on Sr atom at energies up to 10 eV. The necessity of the calibration of the experimental cross sections [20] by shifting energy on 0.98 eV was demonstrated. In the energy dependence of the ICS for elastic scattering and total ICS for $e-$Sr collision were found two maxima: at energies 1.04 eV and 1.86 eV. The first of these corresponds to a powerful $5s^24d[^2D^e]$ shape-resonance in $^2D^e$-wave. The second – is the not fully manifested (due to the opening of new channels of scattering) $5s5p^2[^1D]\ ^2D^e$ resonance.

In [7] listed the results of a study of the elastic scattering and excitation of the neutral silicon by electron impact. The range of collision energies extends from threshold to 100 eV. Prior to our BSR34-calculations of scattering processes $e-$Si, there were no data about their cross sections in the literature. For accurate representation of the wave functions of the Si target atom we used the MCHF-method with non-orthogonal orbitals. They were optimized in independent calculations for each term separately. The close-coupling expansion for the collision wavefunction (9) included 34 bound states of neutral silicon derived from the [Ne] $3s^23p^2$, $3s3p^3$, $3s^23p4s$, $3s^23p5s$, $3s^23p4p$, $3s^23p5p$, $3s^23p3d$, and $3s^23p4d$ configurations, plus seven pseudostates to fully take into account the dipole polarizability of the ground state and the three lowest excited states of atomic silicon (approximation BSR41).

The choice of these bases allowed a fairly accurate description of the most important transitions from the ground $3s^23p^2\ ^3P$ and two metastable $3s^23p^2\ ^1D$

and $3s^2 3p^2\ ^1S$ states of Si atom. Fig. 2 shows the energy dependence of ICS for some major transitions from the ground state of the atom $3s^2 3p^2\ ^3P$ Si. Results were obtained using approximations BSR41 and BSR34. The curves for different scattering approaches are close to each other. Significant differences appear only for some transitions in high-lying states of the Si atom. These differences point to the weak convergence of the strong coupling expansion: for transitions in a high-lying states becomes significant the effects of target continuum excitation, i.e. ionization. Fig. 2 shows that the inclusion of polarization and exchange-correlation effects can lead to a significant change (up to factor 2) of the calculated electron impact excitation cross sections on Si atom.

In [8] were studied the processes of electron scattering on fluorine atom in the collision energy range from threshold to 100 eV. The MCHF method in combination with $B$-spline expansions was used for an accurate representation of the target wave functions. The sensitivity of the results to the coupling of discrete states and the target continuum was checked by comparing the data, obtained in different approximations. The latter differ by the number and selection of basis functions in the $R$-matrix expansion (9). The maximum dimension of the basis in BSR39 approximation was 39 states, while the extensive BSR690 calculation included the CC-39 expansion of the physical states and more than 650 continuum pseudostates. Both correlation and polarization effects are found to be important for accurate calculations of the cross sections. Coupling to the target continuum strongly affects transitions from the ground state, but to a lesser extent the strong transitions between excited states.

$R$-matrix calculations of $e$–F scattering were carried out using BSR-parallelized version code [2]. To represent orbitals of the continuous spectrum $F_{i\alpha}^{\Gamma}$ in the internal region $r \leq 30a_0$ used a basis of 58 $B$-splines of order 8. Another characteristic of these BSR-calculations was the use of orthogonal orbitals. They were used both for construction of the wave functions of the target (3) and for presenting the collision function (9).

Appreciable resonance structure was found in the energy dependence of the cross sections of elastic scattering and excitation. It is caused by the formation and decay autodetachment states (ADS) of the negative fluorine ion $\mathrm{F}^-(2p^4 3lnl')$ $n = 3, 4$, and $l, l' = 0, 1, 2, \ldots$ The properties of these ADS is largely determined by the correlations in the motion of excited electrons. Important factors are also the polarization of the target F and the coupling of discrete states and the continuum. The parameters (position and width) for 24 Feshbach type resonances in $e^{\smile}\mathrm{F}$ scattering were defined, and their spectroscopic classification was held.

The main result of [8] is extensive array of data regarding the characteristics of the electron scattering on fluorine atom. First of all, these are the energy dependencies of ICS for the cases elastic scattering, momentum transfer, excitation, and ionization from the ground state. The excitation cross sections were obtained for all possible transitions between the lower 26 states F; were established significant differences (up to a factor of 2-3 in some energy ranges) between results of BSR39- and BSR690-models. This indicates slow convergence of the CC-expansion for $e$–F scattering. It has been revealed the strong influence of the interaction of discrete states and the continuum of the target on the excitation cross section.

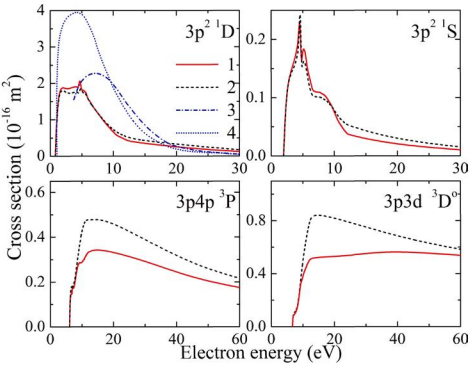


Figure 2: The ICS of some transitions from the ground $3s^2 3p^2\ ^3P$ state of the Si atom: 1, 2 – calculations in approximations BSR41 and BSR34 [7] with and without polarizational pseudo-states, respectively; 3, 4 – calculations by other authors in distorted waves method for transition $^3P \to ^1D$ (see [7])

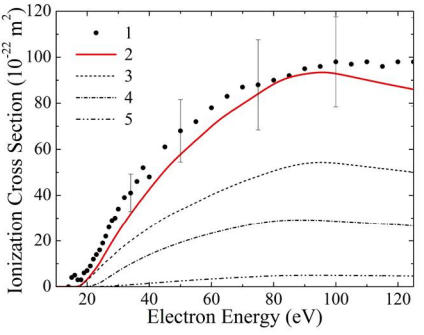


Figure 3: Cross section for electron-impact ionization of fluorine from the $2s^2 2p^5\ ^2P^o$ ground state. 1 – experimental data of Hayes *et al.* [21]; 2 – the our BSR690 results [8]; 3, 4, 5 – BSR690, partial cross sections for $2p^4\ ^3P$, $^1D$ and $^1S$ states of $F^+$

This is particularly evident at intermediate energies collision. That is, the availability of unfilled $2p$-subshell of F atom significantly affects on inelastic $e-$F collision cross sections. In a study [8] we for the first time calculated the electron impact ionization cross section of the F atom. The BSR690-calculation results (Fig. 1) are in good agreement with the available experimental data [21].

The calculations of electron scattering on two more atoms: boron [9] and aluminum [10] have been performed by us in approximations BSR28 (for B) and BSR32, BSR81, BSR587 (for Al). Unfortunately, the limited scope of this review do not allow us to discuss the results of these studies.

# 4 Conclusion

We have presented the general principles and ideas, underlying in the $B$-spline $R$-matrix method (BSR) [2] with a non-orthogonal orbitals. Various examples of the application of BSR method to problems of atomic structure, electron collisions and photodetachment processes were given. The use of non-orthogonal single-electron orbitals eliminates orthogonal restrictions imposed in many other theoretical approaches. These restrictions are intended only for the convenience of calculation, rather than for reasons of physical necessity. Rejecting the orthogonality conditions, BSR method significantly improves the accuracy of the target description. Accordingly, it becomes possible to further accurate calculation of the collision processes.

From a numerical point of view, key ingredients of the method are the $B$-splines that represent the orbitals of the active target electrons as well as the projectile, if necessary.

We also investigated the role of coupling effects between discrete states and the target continuum at the excitation and ionization of atoms by electron impact. The necessity of taking them into account in the calculation of scattering characteristics ($e$−Si, $e$−F and $e$−Al) is showed. A strong sensitivity of the scattering cross sections to the effects of electron correlation both in the $N$-electron target atom, and in the $(N + 1)$-electron collision system is revealed. For each of the above atoms was obtained a large set of systematic data related to the EA-collision characteristics, that have considerable practical interest.

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