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ELECTRON SCATTERING BY THE BORON ATOM

The *B*-spline *R*-matrix method (BSR) has been applied to study the electron-impact excitation of the neutral boron atom with the energy range from threshold up to 60 eV. The multiconfiguration Hartree-Fock method with nonorthogonal orbitals was used to generate and represent precisely the target wavefunctions. The present close-coupling expansion includes 28 bound states of neutral boron: 8 states are lower than the first ionization threshold and 20 states above than this threshold. The excitation integral cross sections are presented for important transitions from ground state. The present BSR results are compared with other theoretical predictions.

Keywords: the boron atom, electron scattering, the *B*-spline *R*-matrix method, integral cross section, resonance structure.

Introduction

Precise cross sections data for electron impact excitation of neutral boron are required to realize the program of controlled thermonuclear fusion. The boronization of the plasma exposed surfaces of tokamaks has proved to be an effective way to produce very pure fusion plasmas (see for example, [1, 2]). Moreover, a surface of walls and internal elements of chambers in tokamaks are subject to strong erosion, and for progress to be made in understanding the erosion of low *Z* materials such as Be, B and C in the next generation of fusion experiments, transport modeling requires complete and accurate electron-impact excitation data for these elements not only from the ground states, but also from the excited states. For beryllium and carbon complete set of calculations for all excitation and ionization rates [3, 4] or excitation cross-sections [5] has already been carried out. Though the electron shell of boron atom containing only five electrons relates to the elementary structure, electron-impact excitation cross sections for boron experimentally are not determined. The basic obstacle for carrying out such experiments is the high temperature of fusion of boron, for this reason no systematic experimental data on electron scattering cross sections for boron atom are available up to date. Unique experimental measurements of cross sections of electron transitions $2s^22p\ ^2P^\circ$ - $2s^23s\ ^2S$, $2s^22p\ ^2P^\circ$ - $2s2p^2\ ^2D$ were carried out using the crossed electron - atomic beam method in 1981 by Kuchenev and Smirnov [6], and reliability of the received results causes the certain doubts. Of theoretical data only three calculations [7-9] meet, in our opinion, the modern criteria of the approach accuracy and systematic character. Both calculations have been carried out with different *R*-matrix method implications with the pseudostates (RMPS). In work [8], the 640 term close-coupling calculation included three distinct pseudostate expansions. It has allowed authors to receive converging structure for three active open-shell electrons, and also accurately represent the high Rydberg and target continuum states. In this work, the derived Maxwell-averaged effective collision strengths were employed to model the spectral emission from boron, which is of importance as for current (TEXTOR) and future (ITER) magnetic fusion reactors.

But when the standard *R*-matrix approach is applied, the non-physical structures the so-called “pseudo-resonances", often arise. An important aspect with regard to the occurrence of pseudo-resonances is the need for a consistent description of the *N*-electron target and (*N*+1)-electron collision problem. Inclusion of many target states in the close-coupling expan-

sion controlled the large number of pseudo-resonances that distort the results in calculations where the N-electron target and the (N+1)-electron collision problem are not treated consistently. The latter problem typically originates from the amount of correlation needed in the description of the target states alone, i.e. it then becomes difficult to keep the matrix dimensions to a tractable size after coupling one more electron to all the target configurations. There is no unique recipe for achieving this goal, but a good approximation is obtained if one additional electron is coupled to very important configuration in the target description. The purpose of the work reported here was to perform independent calculations for the low-energy electron scattering from neutral boron, using highly accurate target wave functions and significantly extended close-coupling expansions compared to previous works [7-9].

Computational methods

A. Structure calculations

Numerical calculations for the present work were performed with a well-known *B*-spline *R*-matrix (BSR) program [10], which was already applied very successfully in detailed investigations of C [5] and Ca [11]. The key feature of this approach is to significantly improve the target description by using compact configuration-interaction expansions involving non-orthogonal sets of term-dependent one-electron orbitals. The possibility to apply the non-orthogonal orbitals to represent both the bound target wave-function and the continuum wave function of the (N+1)-electron scattering problem is a specific feature of the BSR-package. In this case construction of the multi-electron basis of the configuration state functions (the so-called CSF-basis [12, 13]) used to expand the wave function of non-relativistic Schroedinger equation for atom is the most complicated stage of implementing the method used. In the present approach, we chose to include the core-valence correlation *ab initio* by adding target configurations with an excited states. This allows us to optimize the atomic wave functions for different states independently, resulting in more accurate target descriptions than those used in previous collision work.

The target states of boron in the present calculations were generated by combining the multi-configuration Hartre-Fock (MCHF) [12-13] and the *B*-spline box-based close-coupling methods [14], since direct MCHF calculations in this case usually lead to very large expansions, which can hardly be used in subsequent scattering calculations. First, we have performed independent MCHF calculations to generate core orbitals for the $1s^2 2s$ ground state of B^{2+} ion and then obtained valence $2p$, $3p$, $3s$, $4s$, $3d$, $4p$, $5s$, $4d$, and $5p$ orbitals from a frozen-core calculation. This yields accurate wave functions with compact multi-configuration expansions, but with nonortogonal orbital sets for individual states. Next, we simulated the core-valence correlation by adding the $2s3\overline{m}$ configurations through the expansion where the over bar indicate a correlated rather than a physical orbital. In this way the Hartree-Fock wave functions $2s3\overline{m}$ were improved by correlation functions χ with a $2s$-excited core. The core-valence correlated states of B^+ were then used as target states in *B*-spline bound-state close-coupling calculations to generate the low-lying states of atomic boron. The final corresponding multichannel expansions for the target had the structure:

$$\Phi\left(2s^2 nl, LS\right) = A\sum_{i,L',S'}\left\{\phi\left(2s^2, L'S'\right)P\left(n_i l_i\right)\right\}^{LS} + \\ + A\sum_{i,L',S'}\left\{\phi\left(2s2p, L'S'\right)P\left(n_i l_i\right)\right\}^{LS} + \\ + \sum_{i,L',S'}\chi\left(2sn_i l_i\left(L'S'\right)n_i' l_i'\right) \tag{1}$$

where A denotes the antisymmetrization operator. The first sum is responsible for the long-range correlation, whereas the second sum contains the short-range correlation terms. For brevity of the notation, we assume that the expansion coefficients are incorporated in the unknown functions $P(nl)$ for the outer valence electron. These $P(nl)$ functions were expanded in a *B*-spline basis, and the corresponding equations were solved subject to the condition that the wave functions vanish at the boundary. This scheme yields a set of orthogonal one-electron orbital for each bound state, but orbi-

tals in different sets are no orthogonal to each other, i.e., we directly include term-dependent effects in our target wave functions. The number of physical states that we can generate in this method depends on the size a of the R-matrix box. Choosing $a = 60a_0$ (a_0 denoting the Bohr radius), we obtained a good description for all included low-lying states of B up to $2s7d^2\,^2S$.

Table 1

Comparison between present (*ab initio* calculated) and observed [15] excitation energies of physical and pseudo states of boron included in the close-coupling expansion (in eV)

№	State	E_{exit} NIST, [15]	E_{exit} BSR28	ΔE_{exit} BSR28	ΔE_{exit} RMPS [9]
1	$2s^22p\,^2P^o$	0.0013	0.0000	0.0013	0.0013
2	$2s2p^2\,^4P$	3.5803	3.5452	0.0352	0.0294
3	$2s^23s\,^2S$	4.9643	4.9859	-0.0216	-0.0287
4	$2s2p^2\,^2D$	5.9335	5.9358	-0.0022	-0.0663
5	$2s^23p\,^2P^o$	6.0273	6.0140	0.0132	0.0138
6	$2s^23d\,^2D$	6.7903	6.7217	0.0686	0.0014
7	$2s2p^2\,^2S$	7.8805	7.8678	0.0128	
8	$2s^26d\,^2D$	7.9158	8.3592	-0.4434	
9	$2s2p^2\,^2P$	8.9924	9.0446	-0.0521	
10	$2s2p3p\,^2D$a	10.8559	10.9474	-.0915	
11	$2s2p3d\,^2D^o$	11.5677	11.1127	0.4550	
12	$2s2p3p\,^2P$	10.7696	11.6179	-0.8483	
13	$2p^3\,^4S^o$	12.0393	12.0324	0.0070	
14	$2p^3\,^2D^o$	12.3736	12.7290	-0.3554	
15	$2p^3\,^2P^o$	13.7808	14.8666	-1.0858	
16	$2s2p3p\,^2S$		15.7284		
17	$2s^25d\,^2D$		16.1692		
18	$2s2p3p\,^2D$ b		16.3402		
19	$2p^27d\,^2P$ a		22.1128		
20	$2p^23s\,^2S$		23.4600		
21	$2p^27d\,^2P$ b		23.9232		
22	$2p^23p\,^2P^o$		24.5191		
23	$2s2p7d\,^2D^o$		24.5734		
24	$2p^23d\,^2D$		25.6681		
25	$2s7p^2\,^2S$		26.2965		
26	$2s2p3d\,^2P^o$ a		27.7505		
27	$2s2p3d\,^2P^o$ b		29.0855		
28	$2s7d^2\,^2S$		36.0046		

Along with the physical states, the above scheme also provides a set of pseudo-states. Keeping sufficient channels in the above close-coupling expansion (1) then allowed us to include the valence correlation. Of course, since the above B-spline bound-state close-coupling calculations generate different nonorthogonal sets of orbitals for each atomic state, their subsequent use is somewhat complicated. The present close-coupling expansion included the eight bound states of neutral boron atom derived from the configurations $1s^22s^22p$, $1s^22s2p^2$, $1s^22s^23l$ ($l = 0, 1, 2$), plus twenty pseudo-states. The target states included in the present scattering calculations are given in Table 1, where we also compare the calculated binding energies with the experimental values. The overall agreement between experiment and theory is fairly good.

B. Collision calculations

For the scattering calculations we employed the B-spline R-matrix code [10], in which a B-spline basis is also used to represent the continuum functions in the internal region. The principal advantage of B-splines is that they form an effectively complete basis, and hence no additional correction to the R-matrix is needed in this case. The amplitudes of the wave functions at the boundary, which are required for the evaluation of the R-matrix, are given by the coefficient of the last spline, which is the only nonzero spline at the boundary. The other important feature of the present code concerns the orthogonality requirements for the one-electron radial functions. We do not impose any orthogonality conditions for the one-electron radial functions used to represent the different target states, and the continuum orbitals do not have to be orthogonal to the bound orbitals either. This allows us to optimize the atomic wave functions for different states independently, resulting in more accurate target descriptions than those used in previous collision calculations [7-9]. The latter may lead to extensive multiconfiguration expansions, especially when correlated pseudo-orbitals are employed to improve the target states. The number of B-splines and the R-matrix radius in the scattering calculations were chosen the same as in the calculation of the target bound states.

The R-matrix radius was set to 60 a_0, where a_0 denotes the Bohr radius. This is sufficiently large for all bound orbitals to be effectively zero at the boundary. We calculated partial waves up to L=15 numerically, with 86 B-splines for the expansion of the continuum orbitals. For the spinallowed transitions, a top-up procedure was employed to estimate the contributions to the cross section from higher L values that were not calculated explicitly. The calculation for the external region was performed using the flexible asymptotic R-matrix (FARM) package [16].

Results and discussion

Cross sections as a function of energy for the most important transitions from the ground $2s^22p\ ^2P^o$ state are presented in Figs. 1–2, in comparison with the results presented by Marchalant et al [8]. Results for angle-integrated cross-sections are compared with experimental data Kuchenev and Smirnov [6] and predictions from other R-matrix calculations [7-9].

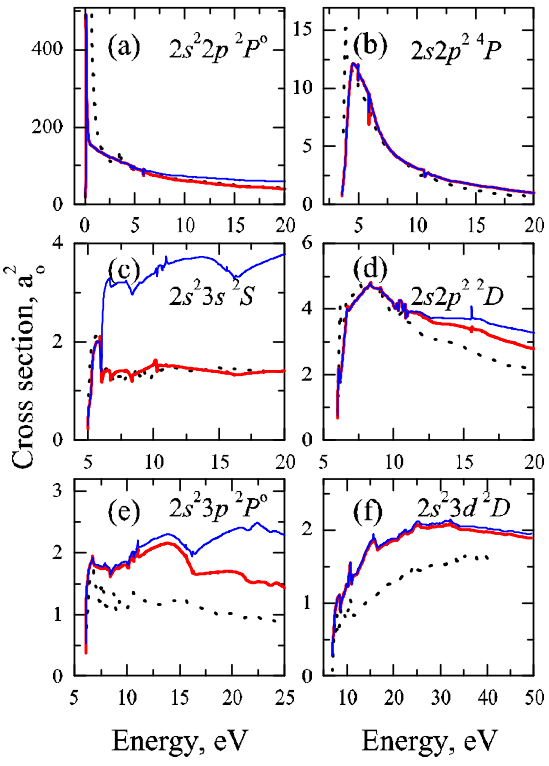

Fig. 1. Electron-impact scattering cross sections from B atom in ground $2s^22p\ ^2P^o$ state: (——) BSR28; (——) BSR28+cascades; (- - -) Marchalant *et al* [8]; final transition states has shows in layers

Our predictions for the angle-integrated cross sections show some discrepancies with those from previous calculations carried out with the standard R-matrix with pseudostates approach in a similar scattering model [7-9]. These discrepancies are mostly due to the different target descriptions, with the present one giving some better agreement with experiment NIST [15] for energy levels. The use of non-orthogonal continuum orbital reduces the pseudo-resonance problem. The excitation cross section exhibit prominent resonance structures in the low-energy region.

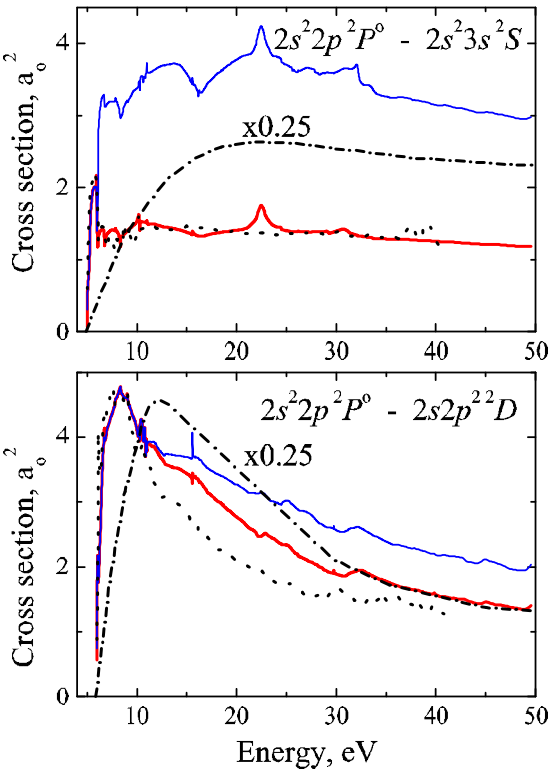

Fig. 2. Electron-impact excitation cross sections from B atom in ground $2s^22p\ ^2P^o$ state: (——) BSR28; (——) BSR28+cascades; (- - -) Marchalant et al [8]; (– · – · –) Kuchenev and Smirnov [6]; final transition states has shows in layers

The present BSR results for low-energy electron scattering for B atoms are shown in Fig. 1 – 2. Note that the BSR code used in the present calculations is less likely to face an imbalance problem. Since we do not impose any orthogonality constraints between the continuum functions and the atomic orbitals, we are not required to compensate for those by adding N+1-electron functions to our close coupling expansion. In practice, this leads to a

substantial reduction in the possible pseudoresonance structure.

This agreement indicates that our *B*-spline expansion includes the principal correlation corrections in the $e^- + \mathrm{B}$ system. The present BSR results are compared with other theoretical predictions and various experimental data. Overall there is acceptable agreement between the present results and those from the *R*-matrix calculations, except for the absolute values.

Summary

We have presented theoretical cross sections for low energy electron collisions with neutral B. The calculations were performed with the *R*-matrix close-coupling method, in which a *B*-spline basis is employed for the representation of the continuum functions. The use of nonorthogonal orbital sets, for both the construction of the target wave functions and the representation of the scattering functions, allowed us to optimize different atomic wave functions independently, and hence to generate more accurate descriptions of the target states than those used in previous collision calculations.

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РОЗСІЯННЯ ЕЛЕКТРОНІВ НА АТОМІ БОРУ

Метод *R*-матриці з B-сплайнами (BSR) був застосований до вивчення збудження електронним ударом атома бору в діапазоні енергій від порогу і до 60 еВ. Для генерування і точного представлення хвильових функцій мішені був використаний багатоконфігураційний метод Хартрі-Фока з неортогональними орбіталями. Даний розклад сильного зв'язку включав 28 станів атома бору: 8 станів, розміщених нижче першого порогу іонізації і 20 станів − розміщених вище цього порогу. Для найважливіших переходів з основного стану представлено інтегральні перерізи збудження. Дані BSR-результати порівняні з іншими теоретичними передбаченнями.

Ключові слова: атом бору, електронне розсіяння, метод *R*-матриці з *B*-сплайнами, інтегральні перерізи.

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РАССЕЯНИЕ ЭЛЕКТРОНОВ НА АТОМЕ БОРА

Метод *R*-матрицы с *B*-сплайнами (BSR) был применен к изучению возбуждения электронным ударом атома бора в диапазоне энергий от порога и до 60 эВ. Для генерирования и точного представления волновых функций мишени был использован многоконфигурационный метод Хартри-Фока с неортогональными орбиталями. Данное разложение сильной связи включало 28 состояний атома бора: 8 состояний, размещенных ниже первого порога ионизации и 20 состояний − размещенных выше этого порога. Для важнейших переходов из основного состояния представлены интегральные сечения возбуждения. Настоящие BSR-результаты сравнены с другими теоретическими предсказаниями.

Ключевые слова: атом бора, рассеяние электронов, метод *R*-матрицы с *B*-сплайнами, интегральные сечения.