INSTITUTE OF EXPERIMENTAL PHYSICS
SLOVAK ACADEMY OF SCIENCES

THE 19th SMALL TRIANGLE MEETING

on theoretical physics

October 15–18, 2017

Medzilaborce

The 19th Small Triangle Meeting on theoretical physics was supported by grant of Plenypotentiary of Slovak Republic in the Joint Institute for Nuclear Research in Dubna.

Published by the Institute of Experimental Physics,
Watsonova 47, 040 01 Košice, Slovakia

Edited by J. Buša, M. Hnatič, and P. Kopčanský

All articles published in this proceedings were peer reviewed.

ISBN

PREFACE

This proceedings comprises the talks presented at the 19^{th} *SMALL TRIANGLE MEETING on theoretical physics* conference, which was held in Medzilaborce, Slovakia, on October 15–18, 2017.

This year, it was already the 19^{th} STM conference, which is organized annually since 1999.

The aim of the conference is to serve as a forum for meeting between theoretical and experimental physicists from Ukraine, Russia, Finland, Hungary, Czech Republic, Poland and Slovakia, where scientists from different research areas of physics met together. This provided an ideal opportunity to exchange knowledge, ideas and experiences. We believe that it helps us in our future work and that we find joint tasks in the following scientific collaboration.

The scientific programme presented at this year's meeting covered the research areas from solid state physics, through nonlinear dynamical systems, atomic, nuclear, high energy physics to biophysics. The final programme included 31 oral presentations. We would like to thank the authors for their cooperation and we are looking forward for the following STM meeting.

All articles published in this proceedings were peer reviewed.

Editors

Program Committee

Michal Hnatič, Faculty of Science, P. J. Šafárik University, Košice
& Institute of Experimental Physics, SAS, Košice, Slovakia
& BLTP, Joint institute for Nuclear Research, Dubna, Russia
Peter Kopčanský, Institute of Experimental Physics, SAS, Košice, Slovakia
Ján Buša, Faculty of Electrical Engineering and Informatics, TU, Košice, Slovakia
Juha Honkonen, National Defence University, Helsinki, Finland
Volodymyr Lazur, Faculty of Physics, Uzhgorod National University, Ukraine
Alexei Gladyshev, BLTP, Joint institute for Nuclear Research, Dubna, Russia

List of participants

Vitaly Aleksiy, UzhNU, Uzhgorod, Ukraine
Rafal Bielas, Adam Miczkiewicz Univesity of Poznan
Šarlota Birnšteinová, FNS UPJŠ, Košice, Slovakia
Alexander Bogdanov, SPbSU, Sankt Petersburg, Russian Federation
Sergii Burylov, Institute of Transport Systems and Tecnologies, NASU, Dnipro
Leonid Bulavin, KNU, Kyiv, Ukraine
Michal Dančo, IEP SAS, Košice, Slovakia & JINR, Dubna, Russia
Alexander Degtyarev, SPbSU, Sankt Petersburg, Russian Federation
Alexei Gladyshev, JINR, Dubna, Russian Federation
Vladimir Gorev, NRC Kurchatov Institute, Moscow, Russian Federation
Michal Hnatič, UPJŠ & IEP SAS, Košice, Slovakia & JINR, Dubna, Russia
Slavomír Hnatič, UPJŠ & IEP SAS, Košice, Slovakia & JINR, Dubna, Russia
Vladimír Ilkovič, IEP SAS, Košice, Slovakia & JINR, Dubna, Russia
Viktor Khmara, UzhNU, Uzhgorod, Ukraine
Arkadiusz Jozefczak, Adam Miczkiewicz Univesity of Poznan
Katarzyna Kaczmarek, Adam Miczkiewicz Univesity of Poznan
Georgii Kalagov, FNS UPJŠ, Košice, Slovakia
Miroslav Karbovanets, UzhNU, Uzhgorod, Ukraine
Peter Kopčanský, IEP SAS, Košice, Slovakia
Olexander Kovalchuk, IP, NASU, Kyiv, Ukraine
Gabriela Kozáková, IEP SAS, Košice, Slovakia
Igor Kudzej, Vihorlat Observatory, Humenné, Slovakia
Yuri Kulchitsky, LNP JINR Dubna
Vladimír Lisý, FEE&I TU, Slovakia & JINR, Dubna, Russia
Martin Menkyna, IEP SAS, Košice, Slovakia
Lukáš Mižišin, FNS UPJŠ, Košice, Slovakia
Štefan Molokáč, Technical University, Košice, Slovakia
Elizaveta Nagy, UzhNU, Uzhgorod, Ukraine
Ivan Nebola, UzhNU, Uzhgorod, Ukraine
Olexander Reity, UzhNU, Uzhgorod, Ukraine
Richard Remecký, IEP SAS, Košice, Slovakia
Jan Smotlacha, JINR, Dubna, Russia
Milan Timko, IEP SAS, Košice, Slovakia
Janka Tóthová, FEE&I TU, Košice, Slovakia
Martin Vaľa, FEE&I TU & IEP SAS, Košice, Slovakia
Peter Zalom, IEP SAS, Košice, Slovakia

Contents

Elastic Scattering of Electrons on Fluorine Atom

E.A. Nagy[1], S.V. Gedeon[1], V.F. Gedeon[1], V.Yu. Lazur[1]

[1]*Department of Theoretical Physics, Uzhhorod National University, Voloshina 54, 88000 Uzhhorod, Ukraine*

Abstract

The B-spline R-matrix (BSR) method is used to study electron collisions with neutral fluorine over an energy range from threshold to 110 eV. This method allows to use the term-dependent nonorthogonal orbitals along with B-splines as basis functions. Thus, it provides the effective accounting of electron correlation. The differential cross sections (DCS) of electron impact elastic scattering on fluorine atom in the considered energy range are calculated. The close coupling (CC) expansion included 39 bound states of the F atom. Energy-angular dependences of DCS for the elastic e–F scattering were obtained and corresponding 3D surfaces of DCS were constructed. The behavior of the DCS angular dependences for elastic e–F collisions with energy changing is discussed.

Keywords: fluorine atom, electron scattering, B-spline R-matrix method, scattering differential cross sections, 3D surfaces.

1 Introduction

The needs of practice constantly require systematic data on the characteristics of electron scattering on complex atoms. This, in particular, relates to collision processes e–F. Atomic sections of such processes can also be used for the prediction of the cross sections of various fluorine compounds. However, fluorine is a highly reactive element. Therefore, it is difficult to obtain reliable cross sections for e–F collisions by direct measurements. For the fluorine atom only the ionization cross sections were determined experimentally [1]. The cross sections of elastic scattering, momentum transfer, and electron-impact excitation, required for modeling the plasma, must be taken from theoretical estimates. A review of the researches of electron scattering on fluorine atoms can be found in our (with co-autors) recent papers [2, 3].

Advances in the physics of electron-atom (EA) collisions depend, first of all, on usage by researcher of powerful theoretical methods and appropriate computing powers. One of these approximations is undoubtedly the B-spline R-matrix (BSR) method [4]. It was used by us for a detailed study of the elastic and inelastic collisions of electrons with a number of atomic systems: Ca [5, 6], Mg [7], Sr [8, 9], Si [10], F [2, 3], Al [11, 12], and B [13]. In the calculations of the targets structure [14, 15], the multiconfigurational Hartree-Fock method (MCHF) was also involved.

Using the BSR method [4] in calculations of the EA-scattering characteristics for neutral fluorine [2, 3] we obtained precise integral (ICS) and differential (DCS) collision cross sections. In article [2], the main attention was paid to the investigation of the energy dependences of the ICS for e–F collision. In paper [3] the energy-angular 3D dependences of the DCS for electron impact excitation of five low-lying states $\{2p^4(^3P)3s\ ^{4,2}P, 2p^4(^3P)3p\ ^4P^o,\ ^{4,2}D^o\}$ of the F atom were presented. In this article, we concentrate our attention on the investigation of the angular and energy-angular dependences of the DCS for e–F elastic scattering.

2 The research method

BSR method [4] is quite versatile. It has been successfully applied to structural calculations of atomic systems and 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. The appropriate clarification was made using boundary conditions for the close coupling (CC) equations. Additionally, the different physical effects are taken into account: the electronic correlations, threshold phenomena, channels coupling.

The features of the method for calculating the structural characteristics of the fluorine atom have been elucidated in detail in the papers [2, 3] mentioned above. Thus, the close coupling expansion in the case of F atom contains the different BSR approximations from 39 target states (BSR39) up to 39 target states plus 651 pseudo-states (large-scale BSR690 expansion). Calculations of the fluorine atomic structure were carried out using both the MCHF[14, 15] and the BSR packages [4]. The general theory of the BSR calculations of EA-scattering and description of the computer programs of the BSR package are given in [4].

The results of the BSR39 calculations of the energies of the 39 lower levels of the F atom and their comparison with the NIST data [16] can be found in [2]. As is known, the number of physical states that can be generated in the BSR method depends on the size of the R-matrix box. In the present calculations, this radius was set to $30a_0$, where $a_0 = 0.529 \times 10^{-10}$ m is the Bohr radius. That allowed us to obtain good descriptions of the fluorine states with principal quantum number for the valence electron up to $n = 5$. The errors in the calculation of both the energy levels and wave functions (the oscillator forces) [2] are sufficiently small. They are much smaller than those obtained in calculations of the structure of the F atom by other authors (see [2]). Among the features of the structure of the fluorine atom, we note a large gap between the energy of the ground state of the F atom and the energy of the lowest excitation threshold, which exceeds 12 eV. Such an energy gap exists only for two elements of the periodic table, namely inert gases of helium and neon. Obviously, this circumstance should somehow affect the character of the 3D surface of the energy-angular dependences of the DCS for the processes of elastic e–F scattering.

The calculation parameters of the $(N+1)$-electronic problem of EA scattering in the inner region ($r \leq a$) for the F atom are also described in [2]. The B-spline basis in the present calculations contains 68 splines of 8th order with the maximum interval in this grid of 0.65 a_0. This is sufficient for a good representation of the

scattering electron wave functions for energies up to 150 eV. Direct numerical calculations were performed for partial waves with total orbital angular momenta $L \leq 25$. Taking into account the total spin and parity leads to 156 partial waves overall. A top-up procedure based on the geometric-series approximation was used to estimate the contribution from higher L values if needed. The calculation for the external region was performed using a parallelized version of the STGF program [17].

3 Results and discussion

In the framework of the BSR39 method, we investigated the behavior of the energy-angular 3D dependences of DCS for the elastic scattering of electrons on fluorine atom. These 3D surfaces contain almost complete information about the energy-angular parameters of the scattering DCS. They can be used as a sensitive test for evaluating the accuracy of the performed calculation. The smoothness of the 3D surface of the DCS indicates a sufficient number of the counted terms in the partial-wave expansion. In contrast, the presence of wrinkles and small folded structures on the 3D surface signalizes that the number of partial waves taken into account needs to be increased. In 1, the energy-angular 3D dependences of the DCS for elastic $e-$F scattering are shown.

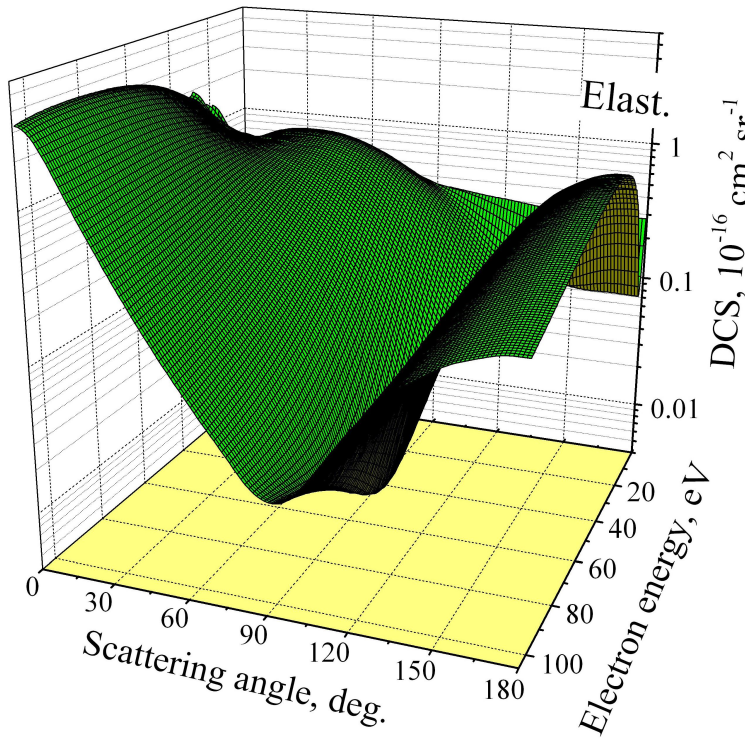

Figure 1: 3D surface of a DCS for elastic scattering of electrons on a fluorine atom

The surface of the energy-angular dependences of the DCS has the form of a deep „canyon" with two smooth gentle slopes. The character of the angular dependences shows that, beginning from an energy of ∼15 eV, the largest contribution to the DCS of the elastic collision is made by scattering at small angles close to the „forward scattering" direction. Fig. 1 also shows that the 3D surface contains a feature localized in the energy-angular plane with a minimum $\sigma = 0.00647 \cdot 10^{-16}$ cm^2 at $[E = 56.415$ eV$, \theta = 100.37°]$, which can be treated as a „critical minimum".

In Fig.2, the angular dependences of the DCS of elastic scattering of electrons on fluorine atom at ten fixed energies are shown. Let us note the considerable variety of the angular dependences of the DCS at different energies for the same transition.

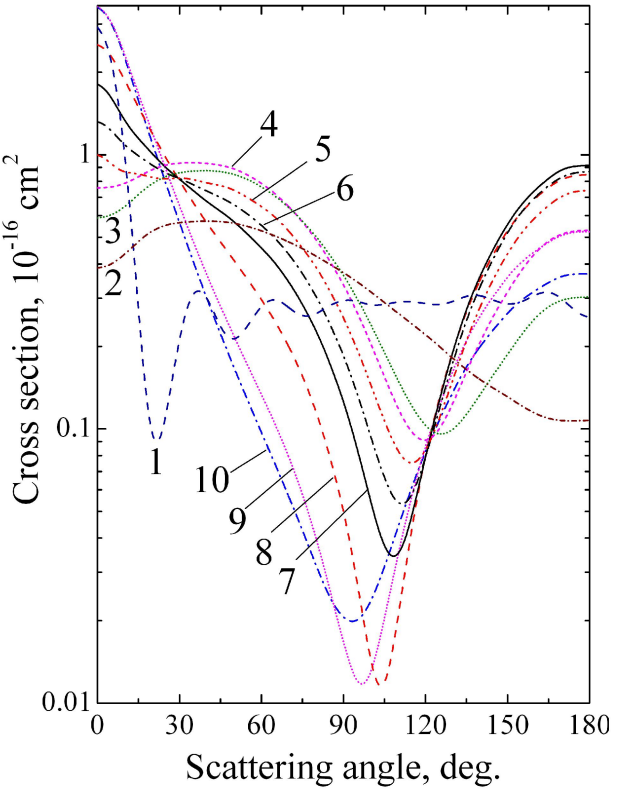

Figure 2: The angular dependences of the DCS of elastic scattering $e-$F at various energies of the incident electron: 1 – 0.011 eV, 2 – 1.99 eV, 3 – 8.99 eV, 4 – 12.67 eV, 5 – 18.10 eV, 6 – 23.69 eV, 7 – 29.80 eV, 8 – 43.54 eV, 9 – 75.37 eV, 10 – 95.78 eV

Summary

We determined the character of the energy-angular dependences of the DCS of elastic $e-$F scattering. It is shown that at energies larger than ~15 eV the main contribution to the collision cross section is made by scattering into small or, conversely, very large angles. The former are close to the direction of "scattering forward", while the latter are close to ~180°. Therefore, the 3D surface of the energy-angular dependences of the DCS has the form of a deep oblique gutter with smooth gentle slopes. An analysis of the angular dependence of the DCS of elastic scattering at fixed electron energies confirms this conclusion. On the discussed 3D surface of the DCS, we also revealed the point of the so-called "critical minimum" [$E = 56.415$ eV, $\theta = 100.37°$]. All this in combination testifies to the complex structure of the investigated 3D surface and the significant role of electronic correlations in its formation.

Acknowledgement

In conclusion the authors wish to express their sincere gratitude to O. Zatsarinny and K. Bartschat for close cooperation and support in the work.

References

[1] T.R. Hayes, R.C. Wetzel, R.S. Freund, *Phys. Rev.A.* **35**, 578 (1987).

[2] V. Gedeon, S. Gedeon, V. Lazur, E. Nagy, O. Zatsarinny, K. Bartschat, *Phys. Rev. A.* **89**, 052713 (2014).

[3] S.V. Gedeon, V.F. Gedeon, V.Yu. Lazur, E.A. Nagy, *Uzhhorod Univ. Scient. Herald. Series. Phys.* **42**, 121 (2017).

[4] O. Zatsarinny, *Comput. Phys. Commun.* **174**, 273 (2006).

[5] O. Zatsarinny, K. Bartschat, S. Gedeon, V. Gedeon, V. Lazur, *Phys. Rev. A.* **74**, 052708 (2006).

[6] O. Zatsarinny, K. Bartschat, L. Bandurina, S. Gedeon, *J. Phys. B.* **40**, 4023 (2007).

[7] O. Zatsarinny, K. Bartschat, S. Gedeon, V. Gedeon, V. Lazur, E. Nagy, *Phys. Rev. A.* **79**, 052709 (2009).

[8] E.A. Nagy, *Uzhhorod Univ. Scient. Herald. Series. Phys.* **25**, 148 (2009).

[9] E.A. Nagy, V.F. Gedeon, S.V. Gedeon, V.Yu. Lazur, *Ukr. Phys. Journ.* **63**, 10 (2018).

[10] V. Gedeon, S. Gedeon, V. Lazur, E. Nagy, O. Zatsarinny, K. Bartschat, *Phys. Rev. A.* **85**, 022711 (2012).

[11] V. Gedeon, S. Gedeon, V. Lazur, E. Nagy, O. Zatsarinny, K. Bartschat, *Phys. Rev. A.* **92**, 052701 (2015).

[12] V. Gedeon, S. Gedeon, V. Lazur, E. Nagy, O. Zatsarinny, K. Bartschat, *J. Phys. B.* **51**, 035004 (2018).

[13] L.O. Bandurina, S.V. Gedeon, *Uzhhorod Univ. Scient. Herald. Series. Phys.* **37**, 49 (2015).

[14] C. Froese Fischer, *Comput. Phys. Commun.* **64**, 369 (1991).

[15] C. Froese Fischer, T. Brage, O. Jonsson, *Computational Atomic Structure. An MCHF Approach* (London: Institute of Physics Publishing, Bristol, 1997).

[16] Yu. Ralchenko, A.E. Kramida, J. Reader, and NIST ASD Team, *NIST Atomic Spectra Database* **version 3.1.5**, (2008), (http://physics.nist.gov/asd3).

[17] N.R. Badnell, *J. Phys. B.* **32**, 5583 (1999).