

EXPERIMENTAL PHYSICS

INSTITUTE OF EXPERIMENTAL PHYSICS

SLOVAK ACADEMY OF SCIENCES



**THE 20<sup>th</sup> SMALL TRIANGLE MEETING  
on theoretical physics**

October 7-10, 2018 | Ptíče

Y OF SCIENCES

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The 20<sup>th</sup> Small Triangle Meeting on theoretical physics was supported by grant of Plenipotentiary 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.

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ISBN

## PREFACE

This proceedings comprises the talks presented at the 20<sup>th</sup> *SMALL TRIANGLE MEETING on theoretical physics* conference, which was held in Ptičie, Slovakia, on October 7–10, 2018.

This year, it was already the 20<sup>th</sup> anniversary of the 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 especially from Ukraine, Russia, Finland, Hungary, Czech Republic, Poland and Slovakia but also from Taiwan, where scientists from different research areas of physics met together. This provides an ideal opportunity to exchange knowledge, ideas and experiences. We are convinced that it helps us in our work and that we find joint tasks in the future scientific collaboration.

The scientific program 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 program included 35 oral presentations. We would like to thank the authors for their cooperation and we are looking forward for the next STM meeting.

All articles published in this proceedings were peer reviewed.

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Tomáš Lučivjanský, FNS P. J. Šafárik University, Košice, Slovakia  
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Milan Timko, IEP SAS, Košice, Slovakia  
Janka Tóthová, FEE&I TU, Košice, Slovakia

# Contents

Š. Birnšteinová, M. Hnatič, T. Lučivjanský, L. Mižišin, V. Škultéty: <i>Turbulent advection of directed percolation process: the effect of compressibility</i>	9
A. Bogdanov, A. Degtyarev, V. Korkhov, T. Kyaw, N. Shchegoleva: <i>Is the Big Data the future of information technologies?</i>	15
Č. Burdík, O. Navrátil: <i>Algebraic Bethe ansatz for RTT-algebra <math>\tilde{\mathcal{A}}_2</math></i>	29
V.V. Gorev: <i>On ball lightning</i>	35
A. Haysak, I. Haysak: <i>On the singular solution of Schroedinger equation</i>	39
M. Hnatič, G. Kalagov: <i>Fluctuation induced first order phase transition in an <math>SU(N)</math> field model</i>	45
M. Hnatič, T. Lučivjanský, L. Mižišin: <i>Tricritical directed percolation: Field-theoretic formulation</i>	57
J. Honkonen: <i>Randomly stirred perfect gas</i>	65
V. Ilkovič: <i>Theory of spin reorientation transition in Heisenberg ferromagnetic system</i>	75
E. Jurčišinová, M. Jurčišin, M. Menkyna: <i>Influence of finite time correlations on the anomalous scaling of passive magnetic fields</i>	85
E. Jurčišinová, M. Jurčišin, R. Remecky: <i>Anisotropic MHD turbulence in space dimensions <math>d \geq 2</math></i>	97
M.V. Khoma, R. Jaquet: <i>On the construction of the non-adiabatic nuclear kinetic energy operator for diatomic and triatomic systems</i>	105
N.Yu. Kondor, E.A. Nagy, S.V. Gedeon, V.F. Gedeon, V.Yu. Lazur: <i>Calculations of the energy structure of neutral phosphorus by B-spline R-matrix method</i>	115
O.V. Kovalchuk, I.P. Studenya, P. Kopčanský, M. Timko, T.M. Kovalchuk: <i>Influence of a liquid crystal with a large magnitude dipole moment of molecules on the dielectric properties of its composites with superionic conductor nanoparticles</i>	123
N. Kučerka, J. Gallová, D. Uhriková: <i>Peculiar properties of lipid membranes affected by water</i>	131
Yuri Kulchitsky: <i>Probing QCD with the ATLAS detector at LHC</i>	139
V. Lackova, P.-Sh. Hu, V.I. Petrenko, N. Tomasovicova, J. Majorosova, C.-L. Zeng, O.I. Ivankov, M.V. Avdeev, P. Kopčanský: <i>Elucidating structures of magnetic nanoparticles-incorporated amyloid fibrils by small-angle neutron scattering contrast variation technique</i>	151
V.Yu. Lazur, S.I. Myhalyna, O.K. Reity, V.V. Rubish, M.I. Karbovanets: <i>Matrix element of the excitation transmission from one two-level atom to another at arbitrary interatomic distances</i>	161
V. Lazur, V. Rubish, O. Reity: <i>Quasiclassical theory of the Dirac equation with a scalar-vector interaction and its applications in the physics of heavy-light mesons</i>	171
V. Lisý, J. Tóthová: <i>Brownian motion under external forces: Modification of the second fluctuation-dissipation theorem</i>	185

I.I. Nebola, A.F. Katanytsia, I.M. Shkyrta, J.M. Pozho: <i>Modelling of complex crystals dispersion laws using <math>3 + d</math> dimensional bases</i> . . . . .	189
O.K. Reity, V.Yu. Lazur, V.M. Khmara, V.K. Reity: <i>Asymptotics of the two-centre wave function in the spheroidal and spherical bases</i> . . . . .	195
A.V. Stadnik, P.S. Sazhin, S. Hnatic: <i>Comparative performance analysis of neural networks in different implementations</i> . . . . .	209
<b>Photo Gallery</b>	<b>213</b>





# Calculations of the energy structure of neutral phosphorus by $B$ -spline $R$ -matrix method

N.Yu. Kondor, E.A. Nagy, S.V. Gedeon, V.F. Gedeon, V.Yu. Lazur

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

## Abstract

The  $B$ -spline  $R$ -matrix (BSR) method is used to study the structure of the electron shell of the neutral phosphorus. 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. In this paper, the energy structure of the phosphorus atom is calculated. The calculation results demonstrate good agreement with the available experimental data. In the future, our data will be used in the study of electron scattering on phosphorus atoms:  $e$ -P.

**Keywords:** atomic systems structure calculations,  $B$ -spline  $R$ -matrix method, manyelectron bases, correlation interaction, phosphorus atom.

## 1 Introduction

Over the past decades, the physics of electron-atomic (EA) collisions has been intensively developed. This is due both to the fundamental nature of the studied processes and applied needs. This is primarily about understanding at a deep level the behavior of submicroscopic, often strongly correlated, quantum mechanical many-particle systems. The result of this understanding is obtaining a large amount of data necessary for modeling the behavior of various types of plasma and discharges, as well as to diagnose their properties. First of all, it concerns the characteristics of the atomic structure, which are used to determine the cross sections and rates of collisions of electrons and photons with atoms and ions.

This work contains a description of the energy structure calculations of the phosphorus atom. These data will be used later to study the electron-atom scattering  $e$ -P. To obtain the characteristics of the atomic structure of neutral phosphorus, we applied the  $B$ -spline  $R$ -matrix (BSR) method [1]. A brief description of this method, which is necessary to understand the calculations we have carried out, is given below. We also present the results of the BSR-calculation of the phosphorus atom structure characteristics. In this paper, we follow the general approach developed in our papers [2]–[11] for BSR-calculations of electron scattering on Ca [2, 3], Mg [4], Sr [5, 6], Si [7], F [8], B [9] and Al [10, 11] atoms.

## 2 The research method

BSR method [1, 12] is quite versatile. It has been successfully applied in the structural calculations of atomic systems, and in 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 is made using boundary conditions for the close coupling (CC) equations. A variety of physical effects are taken into account separately: the electronic correlations, threshold phenomena, coupling channels. Although the BSR method can be applied to heavy atoms, we will work here with the light atomic targets only.

Electron-atom collision theory is concerned with calculation of an  $(N + 1)$ -electron system states, for which  $N$  electrons are bound in an atom or atomic ion and one electron can escape to infinity. Such states may be represented accurately using the close-coupling expansion (1).

$$\begin{aligned} \Psi_{\alpha}^{\Gamma}(x_1, \dots, x_{N+1}) = & \hat{A} \sum_{i=1}^n \bar{\Phi}_i^{\Gamma}(x_1, \dots, x_N; \hat{r}_{N+1} \sigma_{N+1}) \frac{1}{r_{N+1}} F_{i\alpha}(r_{N+1}) + \\ & + \sum_{j=1}^m c_j \chi_j^{\Gamma}(x_1, \dots, x_{N+1}), \end{aligned} \quad (1)$$

where  $\hat{A}$  is the antisymmetrization operator with respect to the exchange of any pair of electrons while  $F_{i\alpha}(r)$  is the radial component of the scattered electron wave function when the target is in the  $i$ th state.  $\bar{\Phi}_i^{\Gamma}$  is called a channel function, which is obtained by coupling the target state  $\Phi_i$  with the spin-angle function of the scattered electron. Let us denote the quantum numbers of the scattered electron in channel  $i$  as  $k_i l_i m_{l_i} m_{s_i}$ . The scattering Hamiltonian  $H_{N+1}$  (see below) is diagonal with respect to the total orbital momentum  $L$ , total spin  $S$ , their projections onto the chosen axis  $M_L$  and  $M_S$ , and the parity  $\pi$  of the total  $(N + 1)$ -electron system.

The Hamiltonian  $H_{N+1}$ , which describes the scattering of an electron on an  $N$ -electron atomic target with the nuclear charge  $Z$ , has the form

$$H_{N+1} = \sum_{i=1}^{N+1} \left( -\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{i>j=1}^{N+1} \frac{1}{r_{ij}}, \quad (2)$$

where  $r_{i,j} = |r_i - r_j|$ ,  $r_i$  and  $r_j$  being the vector coordinates of electrons  $i$  and  $j$ . The origin of the coordinate frame is set at the target nucleus, which is assumed to have an infinite mass. We introduce a set of target eigenstates, and possibly pseudostates  $\Phi_i$ , and their corresponding eigenenergies  $E_i$  by the equation

$$\langle \Phi_i | H_N | \Phi_j \rangle = E_i(Z, N) \delta_{ij}, \quad (3)$$

where the integration is carried out over all the space and spin coordinates of the target electrons. Then the total energy is  $E = E_i + \frac{k_i^2}{2}$ , with  $E_i$  being the energy of the target in the state  $i$  while  $\frac{k_i^2}{2}$ , represents the kinetic energy of the projectile

electron. The target states  $\Phi_i$  are expanded in terms of single-configuration basis states  $\varphi_j$  by

$$\Phi_i(x_1, \dots, x_N) = \sum_j \varphi_j(x_1, \dots, x_N) c_{ij}, \quad (4)$$

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

Therefore, in the expansion (1) it is convenient to use the total momentum representation in which  $\Gamma = \gamma L S M_L M_S \pi$  and the channel functions  $\bar{\Phi}_i^\Gamma$  are defined according to the following coupling:

$$\begin{aligned} \bar{\Phi}_i^\Gamma(x_1, \dots, x_{N+1}; \hat{r}_{N+1} \sigma_{N+1}) = \\ \sum_{M_{L_i} m_{l_i}} \sum_{M_{S_i} m_{s_i}} (L_i M_{L_i} l_i m_{l_i} | L M_L) (S_i M_{S_i} \frac{1}{2} m_{s_i} | S M_S) \times \\ \times \Phi_i(x_1, \dots, x_N) Y_{l_i, m_{l_i}}(\hat{r}_{N+1}) \chi_{\frac{1}{2} m_{s_i}}(\sigma_{N+1}). \end{aligned} \quad (5)$$

Here  $Y_{l_m}$  is a spherical harmonic,  $\chi^{(\sigma)}$  is a spin function, and we use the standard notation for the Clebsch-Gordan coefficients. The function  $F_{i\alpha}(x_{N+1})$  of the incident electron describes both open and closed channels. Very often the  $F_{i\alpha}(x_{N+1})$  in (1) are called channel orbitals. The expansion (1) is also suitable for representing states with one highly excited electron and the other  $N$  electrons that are more tightly bound. When the close-coupling approximation is used to calculate bound states of atomic systems, it is referred to as the frozen-core (FCS) approximation, and the  $\Phi_i$  are usually labeled 'core' rather than 'target' functions. The FCS method has several advantages. It can readily be extended to highly excited states. The energies and wavefunctions can be computed efficiently with a high accuracy. For close-coupling collision calculations can be used the same expansions as for FCS bound-state calculations. Often a comparison of the calculated bound-state energies with experimental energies provides a verification of the accuracy of the collision calculations. At the same time, it is possible to take advantage of the extensive experience accumulated during close-coupling collision calculations and use software developed for such calculations. An example of the FCS method usage for the study of Rydberg series is the calculations made by Burrington and Seaton [13] using the  $R$ -matrix method [14].

The accuracy of the both methods mentioned above is restricted through the use of finite-difference methods for computing the radial functions. More accurate numerical results can be obtained by using a spline FCS method for Rydberg series, in which the wavefunctions of the outer electrons are expanded directly into  $B$ -splines in some finite region  $r \leq a$ , with a sufficiently large value of  $a$ . Such method is implemented in the BSR package [1].

The choice of  $B$ -splines as basis functions has some advantages. The completeness of the  $B$ -spline basis ensures that, in principle, we can study the entire

Rydberg series. The number of physical states that we can obtain in one diagonalization is defined by the box radius  $a$ , which can be varied easily in the  $B$ -spline representation. Exponential grid was found to be quite suitable for bound states, and it allows us to use a rather large radius with a relatively small number of  $B$ -splines.

The wavefunctions in this method are obtained for all radii and for all Rydberg states under consideration. There is no need to obtain an asymptotic solution and to match it to the inner-region solution as in the standard  $R$ -matrix method [14]. This considerably simplifies the calculations and the codes.

Our implementation of the spline method [1] differs from a previous one [15] in that it uses non-orthogonal orbitals, both for the construction of target wavefunctions and for the representation of the outer electron. It provides us a high flexibility in the choice of the 'target' wavefunctions, which can be optimized for each atomic state separately, and also in the addition of different correlation corrections. In the present program, the core-core correlation may be taken into account by using extensive multi-configuration target states. The core-valence correlation can be introduced, basically, in two ways, either by using a large set of excited target states in the close-coupling expansion or by introducing additional  $(N + 1)$ -electron states, specially designed for this purpose.

### 3 Results and discussion

Despite the presence in the literature of a certain number of studies on individual processes accompanying EA-scattering of  $e-P$  (see, for example, [16]), there is a lack of data about the energy structure of neutral phosphorus. Therefore, we have the possibility to compare the energy values of the spectroscopic states of the phosphorus atom only with the experimental data of NIST [17].

**General characteristics of the phosphorus atom spectrum.** The phosphorus atom belongs to the elements of the V group of the periodic system, along with the nitrogen, arsenic, antimony, and bismuth atoms. The core charge is  $Z = 15$ . The configuration of ground state is  $1s^2 2s^2 2p^6 3s^2 3p^3 \ ^4S^o$ . The spectrum of neutral phosphorus, according to NIST [17], fig. 1, is quite complicated. The three lower levels correspond to different terms ( $\ ^4S^o$ ,  $\ ^2D^o$ ,  $\ ^2P^o$ ) of the  $3s^2 3p^3$  ground state configuration with energies of 0.0, 1.4097, and 2.3234 eV, respectively. The value of the  $LS$  energies of the spectroscopic states was obtained due to the weight averaging of the fine structure levels during the transition from the NIST  $LSJ$  representation [17] to the  $LS$  coupling approximation used by us. Note that several lower levels of this spectrum are formed mainly by excitation of one  $3p$  electron from the valence shell to any of the spectroscopic levels of the  $3s^2 3p^2 ({}^3P)nl$  configuration ( $n = 3, 4, 5, 6, 7, l = 0, 1, 2, 3, 4$ ). However, the 6th in order  $LS$ -level  $3s 3p^4 \ ^4P$  is formed by excitation of a  $3s$  electron, and thus it is necessary to consider configurations with vacancies in the inner  $3s$ -shell. There are also serious difficulties in calculating the eighth in order  $3s^2 3p^2 ({}^1D) 4s \ ^2D$   $LS$ -level. It has an intermediate term  $\ ^1D$ , not  $\ ^3P$ , as in other cases. All this requires significant corrections to the calculation of the spectroscopic states of the phosphorus atom.

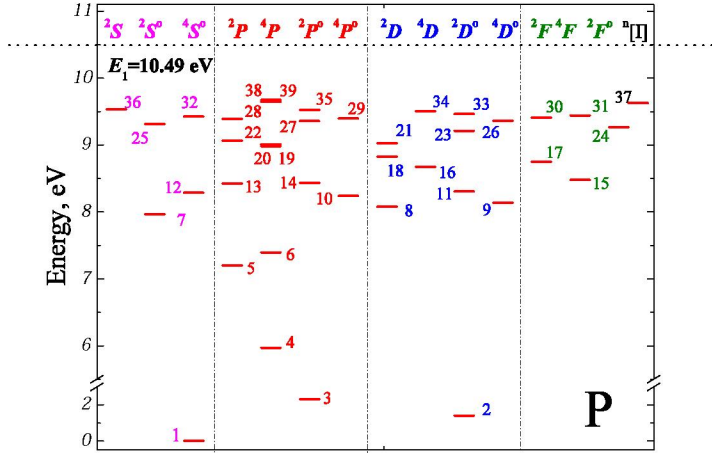


Figure 1: (Color online) Layout of 39 lower  $LS$  energy levels of the phosphorus atom and their distribution over terms according to NIST [17].

First of all, we note that in the lower part of the spectrum of the atom P, there are states with a „unfrozen”  $3s$  shell. This indicates the need to take into account in the calculations both the valence and core-valence correlations. For a more complete considering of the valence correlation, the presence of a stable negative phosphorus ion with a  $3p^4 \ ^3P_2$  configuration and a relative energy of 0.7465 eV should be taken into account. The relatively small charge of the nucleus and the absence of strong splitting of any of the levels on the  $LSJ$  sublevels indicates a relatively small role of relativistic effects.

The main problem in calculating the structure of the target atom and the bond with the continuum for phosphorus is closely related to the  $3s^23p^2(^3P)nl$ . configuration. Orbitals in this configuration must be corrected through interaction with the  $3p^2(^1D)nl$  and  $3p^2(^1P)nl$ . configuration sequences. Note that in the NIST scheme, Fig. 1, a significant part of the phosphorus atom spectrum from the  $3p^2(^1D)nl$  and  $3p^2(^1P)nl$  configurations is not shown, as well as the electronic configurations of the autoionization spectrum placed above.

In the practical calculation of the spectrum of any atom, the set of physical states of this target atom need to be determined first of all. These states will be calculated in scope of approximation chosen from various physical and computational considerations. Such states for the P atom are shown in Table 1.

As shown on Fig. 1 phosphorus atom is characterized by a sufficiently high ionization threshold  $E_{ion} = 10.49$  eV, which exceeds the ionization potentials of the third period elements adjacent to it – silicon (8.15 eV) and sulfur (10.36 eV). However, there is a very narrow energy gap between its ground state of  $3p^3 \ ^4S^\circ$  and the lower excited states of the same  $3p^3 \ ^2D^\circ$  and  $3p^3 \ ^2P^\circ$  configuration. The energies of these states are, respectively, 0.0, 1.4097, and 2.3234 eV, as already mentioned above. In other words, the electrons of the valence  $3p$  phosphorus shell can be excited easily to lower metastable levels. It can also be noted that for the 39 lower configuration states of the phosphorus atom, the number of  $S$ -,  $P$ -,  $D$ - and  $F$ -terms correlates as 6: 16: 11: and 5. Naturally, the accuracy of calculating  $P$ - and  $D$ -terms is decisive in determining of the spectrum of the atom P. Note

Table 1: Spectroscopic states of the atom P under the first ionization threshold (P II  $3p^2$  [ $^3P$ ],  $E_i = 10.49$  eV) are taken into account in this paper

Term	Single electronic orbitals
$^2S$	$3s^23p^2(^1S)4s; 3s3p^4(^1S)$
$^2S^o$	$3s^23p^2(^3P)4p, 5p$
$^4S^o$	$3s^23p^3; 3s^23p^2(^3P)4p, 5p$
$^2P$	$3s^23p^2(^3P)4s, 3d, 5s, 4d, 6s; 3s3p^4(^3P)$
$^4P$	$3s^23p^2(^3P)4s, 3s3d^4(^3P); 3s^23p^2(^3P)5s, 3d, 4d, 6s$
$^2P^o$	$3s^23p^3; 3s^23p^2(^3P)4p; 3p^2(^1D)4p, 3p^2(^3P)5p$
$^4P^o$	$3s^23p^2(^3P)4s, 5p$
$^2D$	$3s^23p^2(^1D)4s; 3s3p^4(^1D); 3p^2(^3P)3d, 4d$
$^4D$	$3s^23p^2(^3P)3d, 4d$
$^2D^o$	$3s^23p^3; 3s^23p^2(^3P)4p; 3p^2(^1D)4p; 3p^2(^3P)5p$
$^4D^o$	$3s^23p^2(^3P)4p, 5p$
$^2F$	$3s^23p^2(^3P)3d, 4d$
$^4F$	$3s^23p^2(^3P)3d, 4d$
$^2F^o$	$3s^23p^2(^1D)4p$

that starting from the 37th level, the main set of spectroscopic levels no longer satisfy the conditions of the  $LSJ$  coupling. Accordingly, this requires a different way to account for the interaction of the orbital and spin moments.

Let us proceed directly to the description of our calculations. According to [1], at the beginning of the BSR calculation of the parameters of the bound states of the P atom, we must calculate the spectroscopic states of the single phosphorus ion  $P^+$ . We obtained these states in the multi-configuration Hartree-Fock approximation [18] using the MCHF software package [19].

Note that in the package [19], the energies of the spectroscopic states are calculated by individual terms. In this case, orthogonalization of all one-electron orbitals within one term is carried out. Generally, the calculation of the energies and wave functions of P I could also be carried out within the framework of the approximation [18]. However, to obtain the accuracy required for scattering calculations, the MCHF method requires the involvement of large number of correlation orbitals. As can be seen from table 1, the usual procedure for MCHF calculations in the case of the phosphorus atom is very difficult. For example, for the  $^4P$  term, it is necessary to calculate single-electron orbitals of the  $3s^23p^2(^3P)4s; 3s3p^4(^3P);$  and  $3s^23p^2(^3P)5s, 3d, 4d, 6s$  configurations; with two different cores  $3s^23p^2(^3P)$  and  $3s3p^4(^3P)$ . That is, two different  $3p$ -orbitals of the neutral phosphorus target core must be taken into account for this term. No less problematic for the calculation are the terms  $^2P^o$  and  $^2D$ . First of all there are state configurations like  $3s^23p^3; 3s^23p^2(^3P)4p; 3p^2(^1D)4p;$  and  $3p^2(^3P)5p$ . Accordingly, it is necessary to take into account three different  $3p$ -orbitals of the target core:  $3s^23p^3; 3p^2(^3P),$  and  $3p^2(^1D)$ . The  $^2D$  term includes the  $3s^23p^2(^1D)4s, 3s3p^4(^1D),$  and  $3p^2(^3P)3d, 4d$  states. Also, it is necessary to take into account three different  $3p$  orbitals of the core: from the  $3s^23p^2(^1D), 3s3p^4(^1D),$  and  $3s^23p^2(^3P)$  configurations.

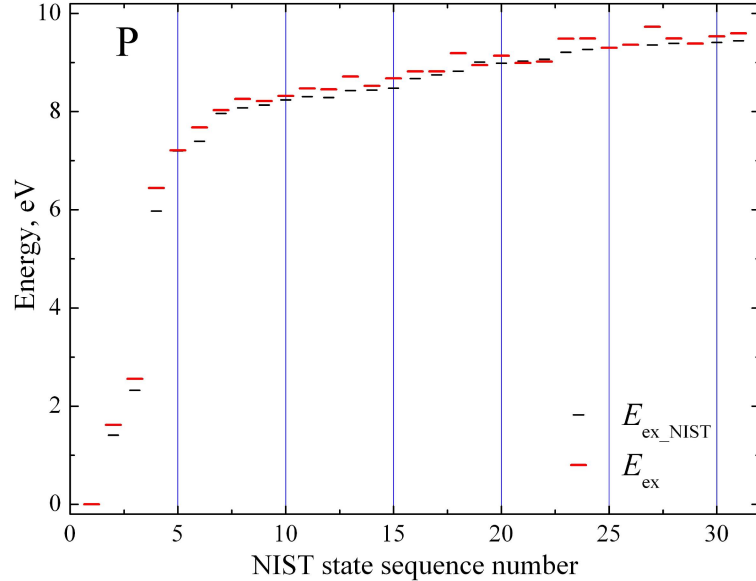


Figure 2: (Color online) The layout of the energy thresholds  $E_{\text{ex}}$  for the P. The results of our BSR calculations are compared with the NIST data [17].

Considering the above, we used the BSR method [1] to calculate the structure of the atomic system P I. This largely saved us from the problems described above, and allowed us to obtain energy and wave functions of the phosphorus atom, suitable for studying  $e$ -P scattering. The procedure of using the software package [1] for calculating bound states is described in Chapter 2.

Figure 2 shows the excitation energies of the  $E_{\text{ex}}$  spectroscopic states that we obtained in a flexible BSR calculation. Their values are compared with experimental data from NIST [17]. It can be seen from the figure that the characteristic accuracy of our BSR results is 0.05–0.2 eV. This is not bad at all, given the objective complexity of the atomic system of neutral phosphorus under study.

## 4 Conclusion

We have presented the general principles and idea, underlying in the  $B$ -spline  $R$ -matrix method (BSR) with a non-orthogonal orbitals. The use of non-orthogonal single-electron orbitals eliminates orthogonal restrictions applied in many other theoretical approaches. These restrictions are introduced purely 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 computational point of view, the 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. As an example, we considered the application of the BSR method to the calculation of the energy structure of a phosphorus atom, that is of considerable practical interest. The calculation results demonstrate good agreement with the available experimental data. In the future, our data will be used in the study of electron scattering  $e$ -P.

## 5 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.

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