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Trends in Computer Science and Information Technology

ENGINEERING GROUP

OPEN ACCESS JOURNAL

ISSN: 2641-3086 Journal DOI: https://dx.doi.org/10.17352/tcsit

Mini Review

ATOM - System for Studying the Structure of Atoms

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Submitted : 24 February, 2023
Accepted : 22 April, 2026
Published : 23 April, 2026

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Keywords: Atom; Ion, Endohedral atom; Photoionization; Decay of vacancies; Many-electron correlations; HF; RPAE; Computer

Abstract

Atomic structure and its study in relationship with radiation are key to the progress of modern physics and associated computational sciences. The growing complexity of atomic systems has led over time to the need to develop effective computational methods that are capable of accurately capturing many-electron interactions and other related processes. The ATOM system is a unified system of computations that attempts to deal with these issues by combining established theoretical methods, such as the Hartree-Fock approximation and the random-phase approximation with exchange.

This mini review gives an overview of the ATOM system, its architecture, its computational capabilities, and its use in modeling atomic processes including photoionization, electron scattering, and decay processes. The hierarchical structure and modular nature of the system allow flexibility in treating a large variety of atomic and ionic interactions and is computationally efficient.

Moreover, the review explains how the ATOM system has evolved over time, how it has helped to support large-scale computational experiments, and how it has helped to reconcile theoretical predictions with experimental results. With all its merits, some aspects of improvement, such as accessibility and integration with contemporary computational environments are also pointed out.

In general, the ATOM system remains an effective instrument of theoretical atomic physics, providing information about the complicated phenomena of atoms and facilitating further studies in the area.

The ATOM system, described in [1-4], contains a large number of programs necessary for calculating atomic processes, including photoionization, Auger and radiative decays, elastic and inelastic scattering, and many others. Calculations are performed within the Hartree-Fock (HF) approximation and the Random-Phase Approximation with Exchange (RPAE), which takes into account the many-electron correlations important in these processes. The ATOM system can be used to perform perturbation theory calculations.

Introduction

The theoretical and computational study of atomic structure and its interaction with radiation has been a fundamental subject of study [1-4]. As the atomic systems have been growing more complex over the decades, more sophisticated computational instruments had to be developed that could provide accurate and efficient results [2,4]. The classical methods of analysis, though basic, tend to be restricted to many-electron systems or strongly correlated processes.

In this regard, computational techniques have become indispensable tools to study the phenomena of atoms [2,5]. They enable researchers to model interactions, make predictions, and test theories with a degree of accuracy which would be hard to obtain experimentally alone. Special program systems that are atomic calculation oriented tools are amongst such tools that are essential in the gap between theory and practice [3,6].

One such initiative is the ATOM system, which has been designed to meet the increasing demands of dependable and

Citation: Ya Amusia M, Chernysheva LV. ATOM - System for Studying the Structure of Atoms. Trends Comput Sci Inf Technol. 2026;11(1):41-45. Available from: https://dx.doi.org/10.17352/tcsit.000108

multifaceted computational frameworks in atomic physics [1-4]. The system by allowing the inclusion of the Hartree-Fock approximation and the random-phase approximation including exchange [2,7,8], allows detailed study of a large variety of atomic processes [7,9,10,11]. Its modular nature and flexibility has enabled it to change over time, to facilitate more advanced calculations.

The scope of this mini review is to present an overview of the ATOM system, the theoretical basis of the system and its impact in the study of the computation of the atomic structure and interactions. The discussion emphasizes its abilities, real-world uses, and its role in the larger framework of quantum mechanical computational devices [5,12].

A system of programs for studying the structure of atoms has been developed, which allows for the calculation of the characteristics of the interaction of atoms and ions with electromagnetic radiation and associated atomic processes with very high accuracy and speed [3,6]. This opened the possibility of conducting corresponding mass calculations and creating tables and databases. Numerical experiments (computer-based calculations within the framework of various theoretical approaches to the physical process under consideration) also allow for comparisons between them, which can be accomplished more quickly and at a lower cost on a computer than a laboratory experiment. All this has allowed, and continues to allow, significant advances in understanding the mechanism of interaction between atoms and ions and electromagnetic radiation, the electronic structure of atoms, and the prediction of new physical effects [4,9,13].

Literature selection method

In this review, it is based on a careful examination of published literature related to the development and application of the ATOM system, as well as foundational studies in computational atomic physics. The primary sources include peer-reviewed journal articles, conference proceedings, and authoritative books that describe both the theoretical framework and practical implementation of the system.

Particular emphasis was placed on works authored by the developers of the ATOM system, as these provide detailed insights into its design, evolution, and capabilities. In addition, relevant studies demonstrating the application of the system to various atomic processes were considered to better understand its practical impact.

To ensure the relevance and completeness of the review, references spanning several decades were included, reflecting both the historical development and more recent advancements in the field. Priority was given to publications that contribute significantly to the understanding of many-electron effects, computational methodologies, and atomic interaction processes.

The selected literature was analyzed with the aim of presenting a coherent overview of the ATOM system while situating it within the broader context of computational tools used in atomic physics research [1-4,6,14-23].

The ATOM system is designed to study the structure of atoms (ions), positrons, muons, endohedrals and the processes occurring with their participation [1-3]. This system provides the user with ample opportunities for applying computational methods in the theoretical study of the electronic structure of atoms, polyatomic formations.

The system implements a method for studying the structure of atoms based on the apparatus of the theory of many bodies. Previous approaches in this area gave results that do not agree well with experimental data [5,24-26].

The ATOM system has been developed since 1965 and is constantly being expanded to include new physical processes [1,2]. This is the first development in the world practice that implements new approaches in the field under study, is user-friendly, easily replenished, uses an interactive mode and shared network resources. It allows you to dramatically increase the level of theoretical research and implement a set of studies called a computational experiment, i.e. processing and testing of various theoretical approaches. The ATOM system allows continuous improvement by incorporating new elements or improving existing ones. Each of the new elements (for example, taking into account relativistic corrections to the motion of atomic electrons) is designed to solve a new physical problem or improve the accuracy of solving previously considered ones. At the same time, the inclusion of new elements does not change the structure of the system, but is its natural development.

The ATOM system allows one to perform calculations in single-electron Hartree (H) and Hartree-Fock (HF) approximations, as well as taking into account many-electron correlations in the Random Phase Approximation with Exchange (RPAE) and its simplified modification (SRPAE). The characteristics found with its help can be the basis for more accurate calculations [1,2,8,27].

The ATOM software package is a system of interconnected programs with a hierarchical structure [2,3]. At the top level there are control programs, each of which solves an independent physical problem. At the lower levels of the hierarchy are applied software modules and a database containing the wave functions of atoms. The system contains more than 70 software modules. The input language belongs to the class of task languages that allow a wide class of physicists who do not have special training in programming to work.

The ATOM system allows solving the following tasks:

1. Calculation of the wave functions in the H and HF approximations: the ground state of the atom; excited states, consistent with the functions of the ground; excited states in a continuous spectrum at given energies in a fixed field of an atom with or without orthogonalization to the wave functions of the ground state; excited states in the discrete spectrum for given values of the principal quantum number in a fixed field of the atom with or without orthogonalization to the wave functions of the ground state; mu meson; positron [1,2,7,9].

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2. Determination of matrix elements of interaction in H and HF approximations, dipole matrix elements of coordinate and momentum operators; Coulomb matrix of effective interaction; matrix elements of the expansion terms of a plane wave in a series in terms of Legendre polynomials; Coulomb matrix elements of various types [1,2,8].

3. Calculation of the characteristics of the processes of interaction of particles with atoms in the HF and RPAE approximations; photoionization cross sections (oscillator strengths) [9,13,28]; coefficients of anisotropy of the angular distribution of photoelectrons [10,11], taking into account the interaction of all electrons of the shell under study, and also taking into account intershell and intersubshell interactions; cross sections for inelastic scattering of fast electrons on atoms [8,27,29]; the probability of scattering of slow electrons by atoms through the self-energy part of the single-particle Green's function in SRPAE [7,30,31]; displacement of the ionization potential compared to its HF value due to the correlation interaction of atomic electrons [24]; the total width of the hole level relative to the Auger decay; characteristics of capture of mu-mesons by atoms [16]; bremsstrahlung spectrum in the approximation of high energies of incident electrons [32]; cross sections for excitation of triplet levels by electrons in the second order of the distorted wave method [25]; dipole dynamic polarizability of an atom, photoionization of endohedrals, inelastic scattering of fast electrons by endohedrals, time delay during photoionization and many others [1,25,33,34].

The first version of the ATOM system was written in ALGOL, the second in Fortran, it is used in UNIX and WINDOWS operating systems, is constantly being improved and developed, experience is being accumulated in its use. All the documentation necessary for the user is presented in the form of manuals (preprints). Each manual contains a physical statement of the problem, a solution method, a description and texts of programs, examples of use.

The ATOM system makes it possible, with a high degree of accuracy, to obtain results on a computer before or without an experiment for many processes associated with the interaction of electrons, photons, and other particles with atoms. The time for calculating the probabilities of one or another process, as compared with the time spent on the corresponding experimental work, is reduced by many times. Widespread use has shown the effectiveness of the ATOM system, which implements the methodology of a computational experiment in studying the structure of atoms [3]. All the results of the calculations that we have carried out since 1969 are collected in the book [3]. The system is widely used by various researchers, about 700 papers have been published in which results were obtained using the ATOM software system, some of which are given in [7,9,10].

The software required to operate the ATOM system can be found in the appendix to [1] in Algol and in [2] in Fortran. These books also contain descriptions of all algorithms and input data for all the programs. The results of a computational experiment using the ATOM system can be found in [4].

Discussion

The ATOM system has established itself as a comprehensive computational framework for studying atomic structure and related processes [1-3,6]. Its strength lies in the integration of well-established theoretical models with a flexible and extensible software architecture *f* [1,2,8]. By combining Hartree-Fock methods with approaches that account for many-electron correlations, the system is able to deliver results that are both accurate and computationally efficient [8,27,29].

One of the key advantages of the ATOM system is its ability to handle a diverse set of atomic phenomena, including photoionization, scattering processes, and decay mechanisms [7,9,13,28,30]. This versatility makes it particularly useful for researchers working across different areas of atomic and molecular physics [31,32,35,36]. Furthermore, the hierarchical organization of the software, along with its modular design, allows users to adapt and extend its functionality depending on the specific requirements of their studies [2,3].

At the same time, it is important to consider the system within the broader ecosystem of computational tools. Several well-established quantum chemistry and atomic physics software packages have been developed over the years, each with its own strengths and areas of specialization [12]. In comparison, the ATOM system offers a distinct focus on atomic processes and many-body effects [1-3,6], which can provide valuable insights in cases where detailed treatment of electron correlations is essential.

Despite its strengths, certain aspects of the system could benefit from further development. For instance, greater accessibility through modern interfaces [14,15], clearer documentation for new users, and integration with contemporary computational environments would enhance its usability [6,15]. Additionally, providing more explicit examples of its application in recent research would help demonstrate its continued relevance in the field.

Overall, the ATOM system remains a significant contribution to computational atomic physics. Its continued development and adaptation will likely play an important role in addressing emerging challenges and expanding the scope of theoretical investigations [3,6,17-23].

Conclusion

The purpose of this article is to give all researchers the opportunity to conduct a computational experiment and, if desired, develop it.

The development of the proposed approach and the creation of the ATOM complex of computational programs continued over 50 years. The development of such systems will make it possible to carry out mass molecular calculations, as well as calculations of atoms placed in strong electric or magnetic

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fields. The obtained results will become the theoretical base, the starting point for comparing theory and experiment. Thus, the area of applicability of the approach that a group of theoretical physicists developed in the theory of the atom will be significantly expanded, providing experimenters with theoretical results of initial approximations that have a relatively high accuracy "on average".

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